PROPERTY RANGES AND CORRELATIONS IN CERAMIC COMPOUNDS

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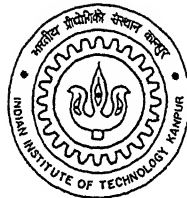JULY, 2001

PROPERTY RANGES AND CORRELATIONS IN CERAMIC COMPOUNDS

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Certificate

3-7-2001

This is to certify that the work contained in the thesis entitled *"Property Ranges and correlations in Ceramic Compounds"* by **Priyanka Awasthi** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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Abstract

In view of the large number of materials available to designers, materials selection in design increasingly relies on materials databases. Often the available information about materials is not complete and one has to use correlations to estimate unknown property values of a specific material .Correlations generally give reasonable results for a class of materials due to similarities in structure, nature of bonding etc.

This work deals with binary ceramic compounds and has the following objectives

- Compilation of property data for binary ceramic compounds
- Develop correlations between various properties
- Develop correlations based on structure maps
- Explore the use of Neural Network techniques in estimating property data

Results have been presented for four classes of binary ceramic compounds. These include borides, carbides, nitrides and oxides.

Dedicated To

Mummy and Papa

(Parents are the representative of GOD)

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Chapter 1

Introduction

1.1 Definition

Ceramic compounds may be defined as products formed with nonmetallic, inorganic materials generally involving high temperatures in their manufacture. The earlier ceramic products were made in the period 4000-1500 B.C. Most of the ceramics are produced from oxides, silicates and refractory materials including aluminides, beryllides, silicides, borides, carbides, nitrides and sulfides.

In general ceramic materials possess a very desirable combination of properties such as high compressive strength, melting point, service temperature, wear resistance, corrosion resistance, low density, low thermal conductivity and specific physical properties (optical, electrical, magnetic). Fig. 1.1 gives a comparison of melting point of various classes of materials for high temperature applications.[1]
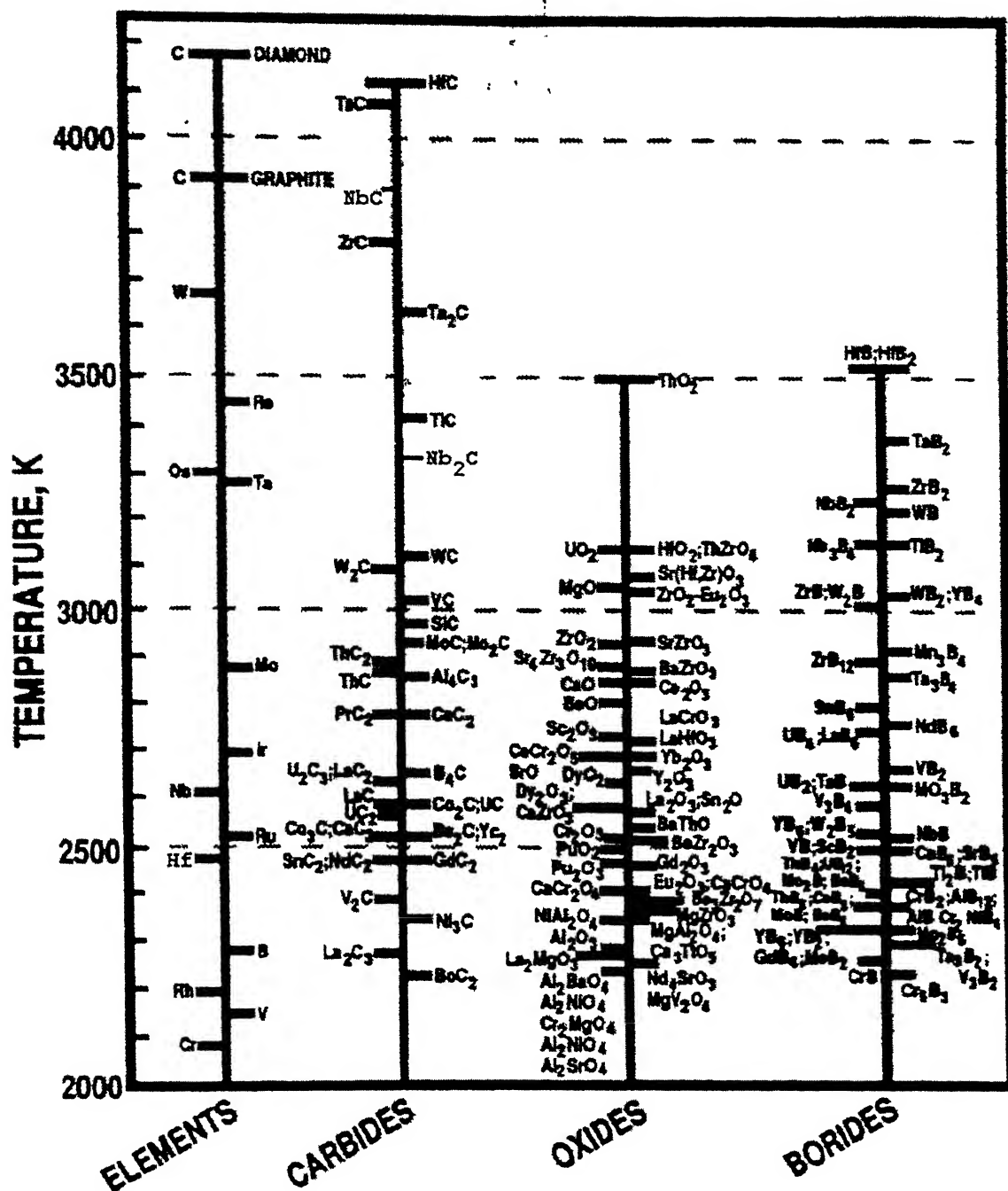
Fig. 1.1 : Melting point of ultra high temperature materials
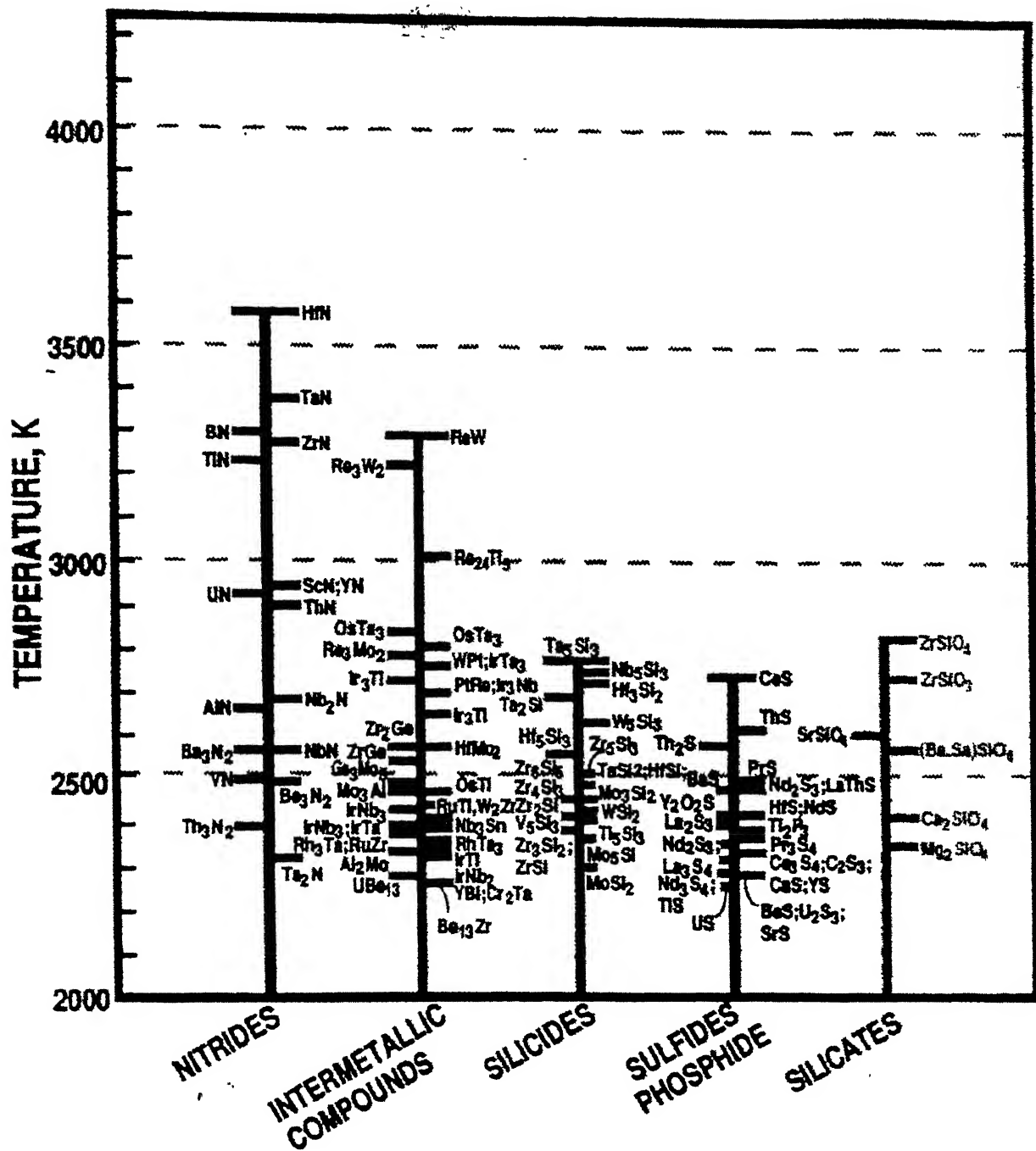
Fig. 1.1(cont.) : Melting point for high temperature materials

Ceramics can be subdivided into different groups under various aspects considering chemical composition, microstructure or application. A possible classification of ceramics is to distinguish between

- silicate ceramics
- oxide ceramics
- non-oxide ceramics

The main feature of silicate ceramics is the glassy phase with a pronounced pore structure. The main content is SiO_2 with additions of Al_2O_3, MgO, BeO ,ZrO_2 etc. While oxide ceramics are distinguished from silicate ceramics by the dominance of a crystalline phase with only a small content of glassy phase.

The non —oxide ceramics comprise:

- elements: carbon in the form of graphite
- nitrides : AlN , BN, Si_3N_4, TiN
- carbides : B_4C , SiC, TiC, WC
- borides : ZrB_2,, TiB_2
- selenides: ZnSe
- sialones: $Si_3 N_4$ with Al_2O_3
- syalons : $Si_3 N_4$ with Al_2O_3 and Y_2O_3

However ceramics have low fracture toughness and tensile strength consequently considerable effort is currently being made to develop new ceramic materials, ceramic based composites with superior properties. Some of the modern day ceramics and their field of utilization are discussed in the Table1.1 [2].

Table1.1: Some applications of ceramics

Application	Ceramic used
Engine manufacturing Utilized properties	Wear resistance, heat insulation, low density, and resistance to corrosion, electrical insulation, and high temperature strength.
Materials	Al_2O_3, Al_2TiO_5, ZrO_2 , SiC, Si_3N_4
Examples	Thermal insulation of combustion chambers valve seats, spark plugs, turbochargers, gas turbines
Industrial processing engineering	

Utilized properties	Resistanceto corrosion, wear resistance
Materials	Al_2O_3, ZrO_2 , SiC,
Examples	Chemical devices, drawing die, sliderings, thread guides, rolls for paper industry
High temperature techniques	
Utilized properties	Resistance to corrosion, thermal insulation, electrical insulation, high temperature strength
Materials	Al_2O_3, ZrO_2, SiC, Si_3N_4 ,BN, C
Examples	Heat exchangers, crucibles, heating conductors
Machining of materials	
Utilized properties	Resistance to corrosion, wear resistance
Materials	Al_2O_3, SiC, Si_3N_4, BN, TiC , TiN
Examples	Cutting tools, grinding wheels, sandblast nozzles
Medical techniques	
Utilized properties	Resistance to corrosion, physiological compatibility
Materials	Al_2O_3, ZrO_2
Examples	Bone replacement, dental ceramics

Thus we see the interest in ceramics arises because of its multidimensional applications varying from pottery to nuclear fuels, from single crystal to molecular sieves and from heat engines to oxygen sensors. [3]

Before we move on to the subject of this thesis we will discuss about the structural properties and applications of some of binary compounds.

1.2   Classes of binary ceramic compounds

Binary compounds are those materials, which are formed of two constituent elements. Some of ceramics under this category are borides, carbides, nitrides and oxides.

1.2.1 Borides

Boron combines with a large number of metals and semimetals to form binary or higher solid compounds. A classification of borides was given by Kisseling [4] on the basis of boron structural elements for various M:B ratios. With increasing M:B ratio the tendency to form boron-boron bonds increases and cross-linked nets, octahedral (MB_6), cubooctahedra (MB_{12}) are formed.

a) The borides are produced by Synthesis from the elements by melting, sintering and hotpressing
b) Borothermic reduction of metal oxide
c) Electrolysis of metal oxide
d) Deposition from the vapour phase

Most of the transition metal boride has melting point temperature higher than 3000^0C .They are used as crucible material for nonferrous metals. Their hardness and wear properties are utilized as thin coatings on metal surfaces, hardness for dodeca and hectoborides are more harder than WC or Al_2O_3. The electrical characteristics cover entire spectrum MB_6, MB_{12} are semiconductors. While NbB, YB_6, ZrB_{12} are superconductors. Lanthanide and actinide borides are best known high temperature electron emitters the lifetime of LaB_6 electrodes is reported to exceed that of tungsten cathodes by twice. CaB_6 is used as a deoxidizer for high conductivity copper. The refractory hexaboride of euporium $(2EuB_6)$ is used as a neutron to control the power of fast breeder reactors [4]

1.2.2 Carbides

Most of the elements form binary compound with carbon. The properties of these carbides are very different so they are classified in four groups

a) Saltlike carbides of metallic elements CaC_2
b) Metal like WC
c) Diamond like B_4C
d) Nonmetal as CO

Saltlike carbides of metallic elements are the carbides of the elements of groups 1-3 and 11-13 of the periodic table. These are transparent and nonelectrical conductors except Lanthanide and Actinide carbides.

Metal like carbides are not attacked by water such as WC, TaC, TiC, NbC most of them are cemented carbides. Their greatest demand is for cutting and drilling tools, mining machinery tire studs scratchproof watchcases. TiC is the hardest carbide but it is too brittle to be used alone.

Diamond like carbides include only Be_4C and SiC they have extreme hardness but it is not used alone industrially because of its decomposition by water. However with some reinforcement silicon carbides are used in stirling heater heads, radomes, infrared domes and in turbine vanes bearings. Similarly TiC is used in turbine disks and in nuclear waste consolidation. Some of carbides and their uses are given as follows

BC

Boron carbide is an exceedingly hard material inferior only to diamond and cubic boron nitride. It has high mechanical strength with low density and high neutron cross-section .Its major use is abrasive grit, lightweight ceramic tiles used in helicopter and monolithic breastplates.

WC

Tungsten carbide is also known as cemented carbide it is used for milling cutters, cutting tips and drills, sawing teeth and blades, drawing and heading dies rolls, nozzles, sealing rings, balls for ball mills, ball for ballpoint pen and for tire studs.

TaC

Tantalum carbide is basically used for long-chipping steel cutting grades. Thermal shock resistance against cratering and oxidation.[5]

1.2.3. Nitrides

Nitrides occur rarely in nature. Titanium nitride has been detected in silicate meteorites as the mineral obsornite. The first industrial application of a nitride was the use of calcium cynamide as a fertilizer. Nitrides can be classified according to their bonding character.

a) The ionic or saltlike nitrides (3rd group element)
b) Covalent nitrides (13-15 group element)
c) Transition metal nitrides
d) Molecule forming nitrides

Nitrides have high degree of hardness, high melting point, metallic luster and superconductivity. *Ionic nitrides* such as Li_3N is a fast ionic conductor. *Covalent nitrides* include BN, AlN, GaN, and SiN. GaN is used as a LED (light emitting diode). Some of more stable transition metal nitrides are used as diffusion barriers in semiconductor technology, solar cells, heat sinks, the surface treatment of windows in microwave technology, Josephson junctions in fast computers, nuclear fusion reactors. Tin is used for magnetic tape heads and fusion reaction insulator; BN is used for transducers special dies. Very thin films of Mo and W nitrides are useful in a number of applications particularly as thin film components such as temperature insensitive precision resistors and capacitors some of these have been prepared by Troitskaya and Pinsker. Nitrides are also known for their comparable high T_c values, a number of high T_c phases of WC and MoC with B1 structure have been found. Some of nitrides and their uses is given as follows

BN

It is second hardest material after diamond so its uses are similar to three of diamond machining and drilling. Dielectric for plasma jet furnace pipes and nozzles for handing liquid metals. Protective tubes and insulating sleeves for thermocouples. In thermal conductivity BN ranks with stainless steel at cryogenic temperatures. It is a lubricant with wide range of temperature.

AlN

It has unusually high thermal conductivity combined with high electrical resistance and a thermal expansion coefficient. So these are used in electrical devices particularly as VLSI. AlN substrates are used as coolers for power transistors, integrated circuits, and laser diodes, thyristors. The crucible surface is coated with AlN to prevent diffusion of impurities from crucible metals into alloys.

SiN

Used in heavy-duty components in automotive engines. SiN bearings can be used up to 1100 ^{0}K. SiN layers are used as diffusion barriers and passive coatings in semiconductor components. [6]

1.2.4 Oxides

The most important oxides are Al_2O_3, ZrO_2, BeO, ThO2, and MgO etc. The properties of single oxides can be modified additives. Their are a large number of oxide ceramic compounds but here we will discuss only few of them.

Alumina

It is a foremost oxide ceramic it is mainly used for sealing disk, printed circuit boards, cutting tools, sandblast nozzles, implants for human medicine, burner nozzles, rotating spindles for accurate machining.

Zirconia

It is used for crucibles, bearing components, manufacture of apparatus, wiredrawing tools, knife blades. Zirconia finds widespread use in a stabilized cubic form as an oxygen sensor.

Beryllia

Beryllia has very high melting point, high heat conductivity. Permanent molds for small metal cast pieces are made of sintered berillia. It is a stable material with respect to radioactive influences. It has a high scattering power to fast neutrons.

Ceria

Ceria belongs to rare group metals. Aluminum, beryllium and all other alkaline metals can be melted in ceria crucibles leaving the metals in a chemically pure state. It is n-type semiconductor. [7]

1.3 Trends in Advanced Materials Data

In the literature and from a design point of view, it is desirable to have information about property data of various materials. In addition it is useful to draw generalizations about trends in material property data for various classes of compound. This is helpful in materials selection as well as estimating missing property data if data of related compound is available.

The first difficulty encountered in searching for generalizations relates to the number of compounds. Given the elements of the periodic table, there are countless combinations that will result in compounds. Table 1.2 shows experimentally known systems, relative to the estimated maximum number of compounds that are grouped by elemental composition. It is taken that the starting number of elements is 100.

Table 1.2: Estimation of materials combinations[7]

Compounds	Maximum number	Experimentally known systems
Unaries	100	100
Binaries	4,950	4000 (81%)
Ternaries	1,61,700	8000 (5%)
Quaternaries	39,21,225	1000 (<0.1%)

In calculating the number of compounds, if one start up with 89 elements and assumes 2 compounds per system (e.g., high temperature, high-pressure phases), the result is 198 unaries, 7823 binaries, 227128 ternaries and 4.8×10^6 quaternaries. Fig. 1.2 shows the distribution of the number of these compounds for which there are crystallographic data: 19597 (48.1%) unaries, 18586 (45.6%) binaries, 19597 (48.1%) ternaries and 1928 (4.7%) quaternaries. These numbers, relative to the estimated maximum number of compounds for each group, shows that binaries are fully investigated, while only 8% of the ternaries have been studied, and research in quaternary field has only just started.
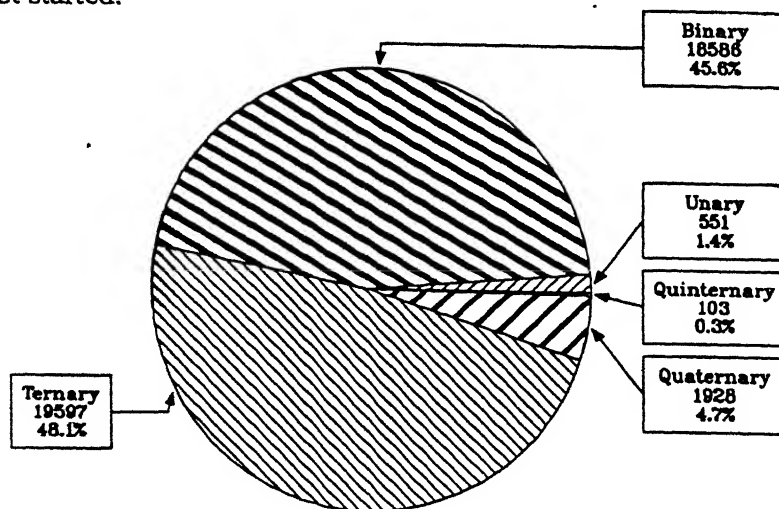
Fig.1.2: Distribution of experimentally known compounds by elemental composition

1.3.1 Properties and Correlations

Material properties of solids lie in a wide range and are characteristic of the class for a given structure and bond-type. Beyond this correlations exist between the values of mechanical, thermal, electrical and other properties based on the nature of bonding and arrangement of the atoms in the material. Some of these correlations can be expressed as

dimensionless groups with much narrower value ranges. This allows one to check the consistency on property values and certain properties can be estimated when values for others are known. Others, which are empirical, can be found by an appropriate search routine. They too can be used to estimate the missing properties, and to assign a reliably range to the estimates [8].

The arrangement of atoms or molecules in space (structure) and the nature of bonding between them determine the properties of solids. Similarities in the properties can be seen in materials with similar structure and bonding. Their values lie within defined ranges, characteristic of the class and are, to varying degrees, interrelated. These relationships can be expressed as dimensionless property groups with nearly constant values for a given class of material [8].

Based on the classification of materials, individual properties of a material class have certain characteristic ranges of values. Certain properties, which originate from the nature of atomic bonding, exhibit strongest correlations and those that are derived from the dependency on defects have less strong correlations. The examples in former case are correlation between modulus and melting point and in later case are strength and toughness. There exist weak correlations when interaction with the environment is involved as in corrosion and wear. There are good reasons for these correlations, which can often be expressed as limits for the values of physically based dimensionless property groups.

The dimensionless property groups take the form

$$C_L < P_1 P_2^n < C_H$$

$$C_L < P_1 P_2^n P_3^m < C_H$$

Where P_1, P_2 and P_3 are material properties, n and m are simple powers, usually -1, $-1/2$, $\frac{1}{2}$ or 1 and C_L and C_H are dimensionless constants represents lower and upper limits between which the property group lies. When such correlations exist they permit checks and estimates, which are more discriminating and precise than do the range checks [8].

1.3.2 Structure mapping

The crystal structures of tens of thousands of binary, ternary and quaternary compounds have been determined since the advent of X-ray crystallography in 1910. To date more than two thousand different types of structure have been identified. The purpose of structure maps is to order this vast empirical data base within two-dimensional or three dimensional plots, so that all compounds with a given structure type are located in well-defined domains which are separated from the domains containing other structure types. The structure maps can then be used for predicting other possible compounds are alloys with a given desired crystal structure. These maps were constructed by choosing coordinates based on those physical factors, which felt to be important in controlling structural stability. For example Villars [9-11] has recently plotted three-dimensional maps (ΔX, ΔR, e/a) for binary compounds with the AB, AB_2, AB_3 and A_3B_5

stoichiometries. The three coordinates reflect the importance of the electronegativity difference ΔX, the atomic size difference ΔR and the average number of valence electrons per atom e/a in determination of structural stability [12,13]. These three dimensional plots suffer several drawbacks. These fairly related to the neglect of the angular dependence of the valence orbitals, since whether the electrons have s-, p- or d-like quantum character is not reflected in the choice of classical coordinates (ΔX, ΔR, e/a).

The alternative approach to the construction of structure maps has been proposed by D.G. Pettifor [14-16], rather than trying to find a set of microscopic coordinates which will produce a separation. The structural types within same n dimensional space, he look instead for a single phenomenological coordinate which would lead to good structural separation of empirical data on binary systems within two dimensions [17].

This was achieved by running a one-dimensional string through the two-dimensional periodic table [12] as shown in Fig. 1.3. Pulling the ends of the string apart orders all the elements along a one dimensional axis, their sequential order being termed the Mendeleev number M. This simple procedure is found to provide excellent structural separation of all binary compounds with a given stoichiometry A_mB_m within a single two-dimensional plot (M_A, M_B). For example AB structure map is shown in Fig. 1.4 & Fig.1.5 shows AB_2 type of structure maps. For other structure maps like AB_2, AB_3, AB_4, AB_5 etc. can be found in Ref. [18]. The values of Mendeleev number and their structure are shown in Table B.1, in Appendix B.
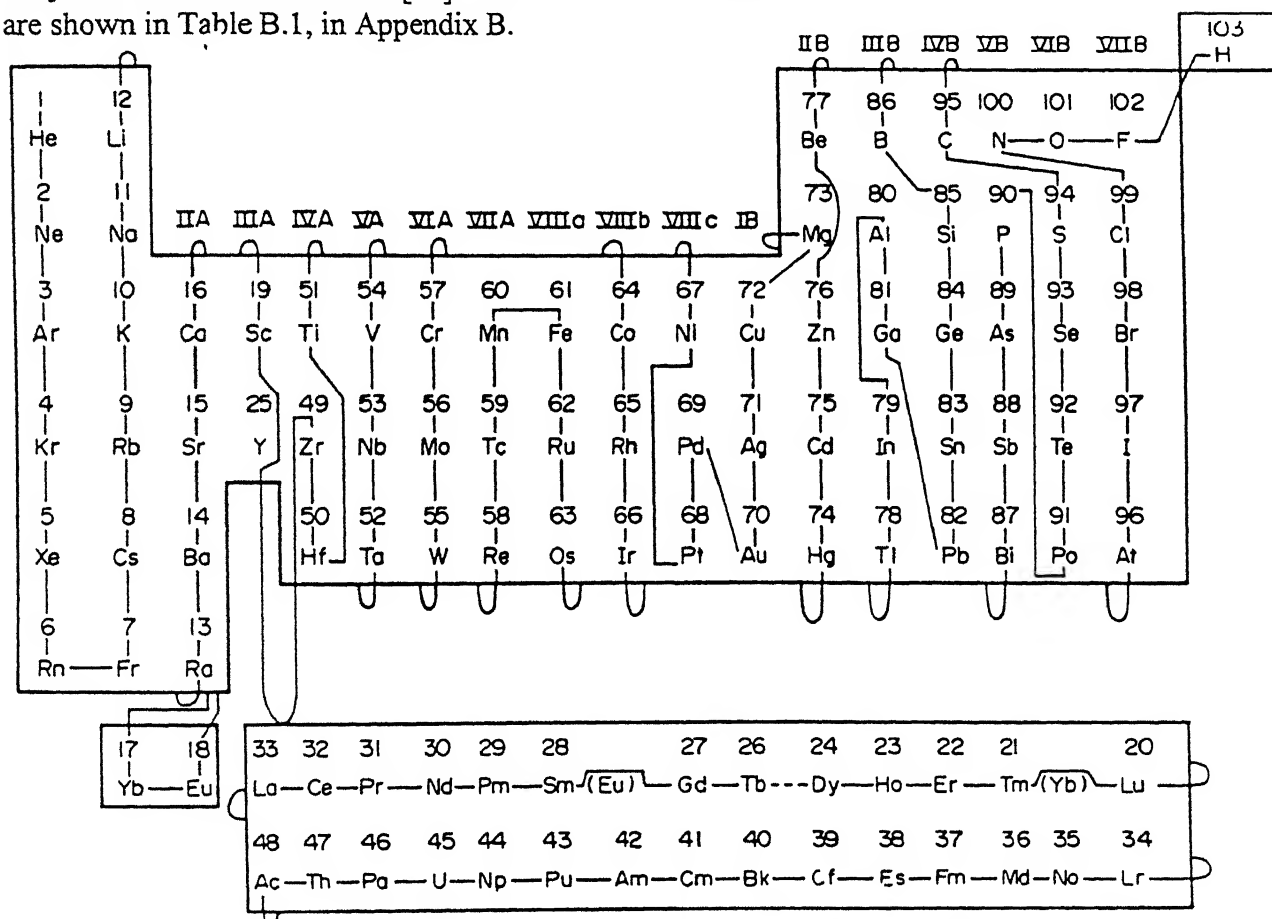
Fig1.3 : Mendeleev number of various elements superposed on periodic table

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1.4 The present work

In terms of materials selection in design there is a need to organize property data so that it can either directly be used in design calculations or may be used to estimate unknown data through the use of correlations. Accordingly, in this work we

- determine various property ranges for binary ceramic compounds
- investigate correlations between various physical properties
- investigate correlations based on structure maps. The later is based on the premise that properties are function of the structure.
- investigate the Neural Network approach for property estimation
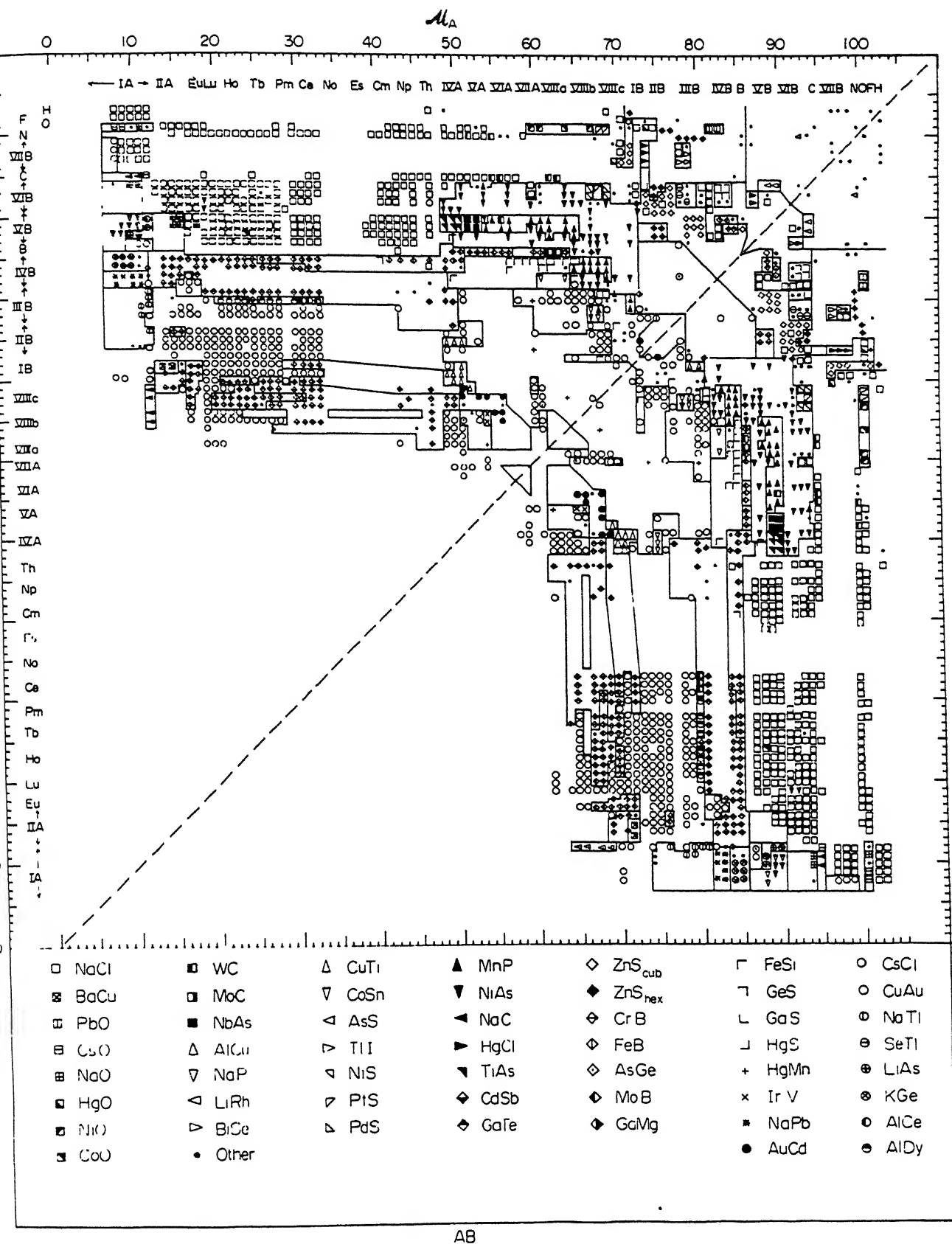
Fig. 1.4: Structure map for AB type compounds
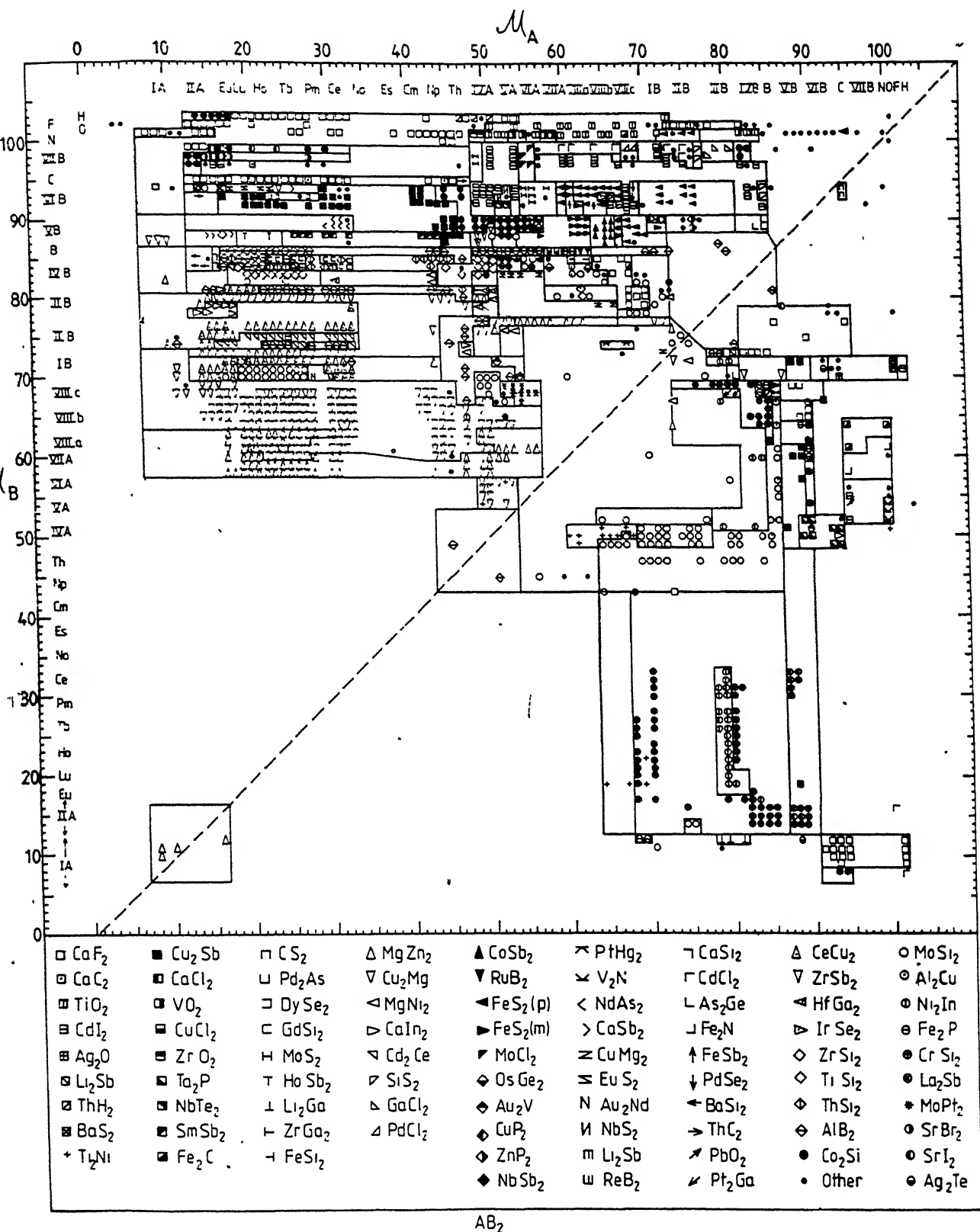
Fig. :Structure map for AB₂ type compounds

Table 1.3: Mendeleev numbers for the elements in the periodic table with their crystal structure [17]

Mendeleev no M	Element	Structure	Mendeleev no M	Element	Structure
1	He	hcp	53	Nb	bcc
2	Ne	fcc	54	V	bcc
3	Ar	fcc	55	W	bcc
4	Kr	fcc	56	Mo	bcc
5	Xe	fcc	57	Cr	bcc
6	Rn	.	58	Re	hcp
7	Fr	..	59	Tc	hcp
8	Cs	bcc	60	Mn	compl
9	Rb	bcc	61	Fe	bcc
10	K	bcc	62	Ru	hcp
11	Na	hcp	63	Os	hcp
12	Li	cp	64	Co	hcp
13	Ra		65	Rh	fcc
14	Ba	bcc	66	Ir	fcc
15	Sr	fcc	67	Ni	fcc
16	Ca	fcc	68	Pt	fcc
17	Yb	hcp	69	Pd	fcc
18	Eu	bcc	70	Au	fcc
19	Sc	hcp	71	Ag	fcc
20	Lu	hcp	72	Cu	fcc
21	Tm	hcp	73	Mg	hcp
22	Er	hcp	74	Hg	rhom
23	Ho	hcp	75	Cd	hcp
24	Dy	hcp	76	Zn	hcp
25	Y	hcp	77	Be	hcp
26	Tb	hcp	78	Tl	hcp
27	Gd	hcp	79	In	tetr
28	Sm	cp	80	Al	fcc
29	Pm	dhcp	81	Ga	compl
30	Nd	dhcp	82	Pb	fcc
31	Pr	dhcp	83	Sn	dia
32	Ce	fcc	84	Ge	dia
33	La	dhcp	85	Si	dia
34	Lr	...	86	B	compl
35	No	..	87	Bi	lay
36	Md	...	88	Sb	lay
37	Fm	..	89	As	lay
38	Es	.	90	P	compl
39	Cf	dhcp	91	Po	sc
40	Bk	dhcp	92	Te	chain
41	Cm	dhcp	93	Se	chain
42	Am	dhcp	94	S	ring
43	Pu	compl	95	C	gra
44	Np	orth	96	At	dim
45	U	orth	97	I	dim
46	Pa	tetr	98	Br	dim
47	Th	fcc	99	Cl	dim
48	Ac	fcc	100	N	dim
49	Zr	hcp	101	O	dim
50	Hf	hcp	102	F	dim
51	Ti	hcp	103	H	dim.
52	Ta	bcc			

sc simple cubic, bcc body centred cubic, fcc face centred cubic, hcp hexagonal close packed, cp close packed, tetr tetragonal, orth orthorhombic, rhom rhombohedral, compl complex, dia daimond, gra graphite, lay, chain, ring and dim are structure types built up from puckered layers, helical chains, rings and dimers respectively.

Chapter 2

Property Ranges in Ceramic Compounds

2.1 Introduction

The conventional classification of engineering materials is generally given by

> Metals and alloys
> Polymers
> Ceramics and glasses
> Composites

Metals have relatively high moduli. We can increase their strength by alloying or by mechanical and heat treatment. These remain ductile and can be used in deformation processes. The general characteristics of these materials are good electrical and thermal conductivity, relatively high strength, high stiffness ductility and shock resistance. These are particularly useful for structural and load bearing applications. Although pure metals are occasionally used, combination of metals (alloys) is normally designed to provide improvement in a particular desirable property.

Polymers have low modulii and strength. They can take large elastic deflection they creep even at room temperature. There properties depend upon temperature and there maximum service temperature is about 200° C. They are very easy to

shape.The large elastic deflections allow the design of polymer components which snap together, making assembly fast and cheap. Polymers are corrosion resistant and they have low coefficient of friction.

Polymers include rubber, plastics and many adhesives. They are produced by creating large molecular structures from organic molecules in a process known as polymerization. Thermoplastic polymers in which long molecular chains are not rigidly connected, have good ductility and formability. Thermosetting polymers are more stronger but more brittle because molecular chains are highly lined.

Ceramics and glasses have high moduli but are brittle when compared to metals. Their brittle compression strength is fifteen times larger than the brittle fracture strength. Their brittleness shows a wide scatter in the strength, depends on the volume of material under load as well as time for which it is applied.They have attractive features of being stiff, hard and abrasion- resistant. They retain their high strength at high temperatures and they are corrosion resistant.

The example of ceramics are brick, glass, tableware, refractories and abrasives, have low electrical and thermal conductivity and consequently are often used as insulators. They have good optical properties also. So they are used in fibre optic system and a variety of devices. They are also used in integrated circuits.

Composite material combineattractiv properties of the constituent materials.They are stiff and strong and they can be tough. Most of the composite materials at present available to the engineer have a polymer matrix. Epoxy or polyster, usually reinforced by fibres of glass, carbon or kelvar. Composite components are extensive and they are relatively difficult to form and join With composites we can produce lightweight, strong, ductile, high temperature resistant materials, shock resistant cutting tools. Advanced aircraft and aerospace engines rely heavily on composites such as carbon- fibre-reinforced polymers.[3]

2.2 Structure - Property Relationships

We consider the properties of a material mainly under two categories

1.Mechanical
2.Physical

Mechanical properties describe how a material responds to an applied force. The most common mechanical properties are strength, ductility and stiffness(modulus of elasticity). However, we are often interested in how a material behaves when it is exposed to a sudden, intense blow , continually cycled by an alternating force i.e. fatigue, exposed to high temperatures (creep), or wear i.e. subjected to abrasive

conditions. Mechanical properties also determine the ease with which a material can be deformed into a useful shape.

Physical properties , which include electrical, magnetic, optical, thermal, elastic and chemical behaviour, which depends on the structure and processing of material. Even small changes in composition cause large scale variations in the electrical conductivity of many semiconducting materials.

The properties of a material depend on its structure. So for example, glassy polyethylene is transparent, whereas crystalline polyethylene is translucent. Imperfections in either type of atomic arrangement may be controlled to produce profound changes in properties.

A grain structure is found in most metals, semiconductors, ceramics and occasionally in polymers. The size and shape of the grain play a key role.In some cases, as with silicon chips for integrated circuits or metals for jet engine parts, it is more reliable to produce only one grain, or a single crystal.

Finally in most materials, more than one phase is present, with each phase having its own unique atomic arrangement and properties. Control of the type size, distributions and amount of these phases within the main body of the material provides an additional way to control properties.

2.3 Classification of properties According to structure

The properties of a material may be classified as:
  (1)   Structure-sensitive
  (2)   Structure-insensitive

The structure insensitive properties are well defined properties of a phase and do not strongly depend on processing history and resultant microstructure whereas structure sensitive properties are dependent not only on the composition and crystal structure of the material but also on structural details that depend upon previous history of the sample. Thus structure-sensitive properties are properties of a particular sample of a material, while the structure insensitive properties relate to the material. Different samples of the same material have essentially identical structure-insensitive properties, but structure-sensitive properties are identical only when the previous treatment has been equivalent. Some of the structure sensitive and structure insensitive properties are shown in Table 2.1

Mechanical properties

The application of a stress to a material may cause many changes.
Elastic deformation, in which strain appears and disappears simultaneously with the application and removal of the stress.

Anelastic deformation, in which strain reaches its maximum value after the stress has reached its maximum value and in which strain disappears after the removal of stress.

Plastic deformation, in which strain occurs simultaneously with the application of the stress, but does not vanish if the strain is removed.

Creep, in which non recoverable strain occurs, while the stress is held at a fixed value.

Fracture, in which separation takes place.

Of these properties, only first (elastic behaviour) is structure-insensitive anelasticity and creep would not be expected to occur in a perfect crystal and plastic deformation and fracture would occur in a perfect crystal at much higher stresses and strains than are normally found experimentally. These four properties are therefore structure sensitive and must be considered in relation to crystal that are imperfect.

Elastic modulus is defined as the slope of the linear elastic part of the stress-strain curve. In reality, moduli measured as slope of stresses are inaccurate, because of the contribution of anelasticity and other factors. Accurate moduli are measured by exciting the natural vibrations of a beam or wire, or by measuring the velocity of waves in the material.

Table 2.1: Classification of properties according to structure

Property	Structure-Insensitive	Structure-Sensitive
Mechanical	Elastic moduli	Fracture strength Plasticity Fracture toughness Creep strength
Physical Thermal	Density Thermal expansion Melting point Thermal conductivity Specific heat Emissivity	
Electrical	Resistivity(metallic) Electrochemical potential Thermo electric properties	Resistivity (Semiconductor and at low temperature)
Magnetic	Paramagnetic and Diamagnetic properties	Ferromagnetic properties
Optical Nuclear	Reflectivity Absorption of radiation	

Anelastic deformation, in which strain reaches its maximum value after the stress has reached its maximum value and in which strain disappears after the removal of stress.

Plastic deformation, in which strain occurs simultaneously with the application of the stress, but does not vanish if the strain is removed.

*Creep ,*in which non recoverable strain occurs, while the stress is held at a fixed value.

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Optical Nuclear	Reflectivity Absorption of radiation	

Physical properties

Density of a crystal can be calculated from the mass of the atoms and geometry of the crystal. The latter one is described by the volume of unit cell of the structure and number of atoms per unit cell. These two parameters in turn depend on the type of the structure and ionic radius appropriate to the structure.

Melting temperature is the most useful structure-insensitive property because
1 Its relative magnitude is a reasonable first approximation to the stiffness of a material since the elastic moduli have a strong correlation with melting temperature
2 In all models of strengthening, values of flow stress increases with the magnitude of elastic constants which in turn increase with T_m.
3 Expansion coefficients are also vary inversely with T_m.
4 It gives some idea about the maximum service temperature of a material.

2.4 Property Ranges for various Category of Materials

A general idea about property ranges of materials is useful in mechanical design. For example, ceramics are hard and brittle, metals are ductile and conduct well, polymers are light and have large expansion coefficients. Chemical engineers strive to survive materials in corrosive condition. Automobile engineers desire lightweight and durable materials. Aerospace engineering demand lightweight materials that perform well both at high temperatures and in the cold vacuum of outer space. The property ranges for various categories of materials are shown in Table 2.2 . Such information has been found very useful for materials selection in design. For example, Fig. 2.1 presents the materials selection map based on elastic modulus and density of various materials[24] . When this information is presented in terms of property ranges, different classes of materials occupy different regions on the plot. The material which offers the best combination of properties can then be located on such maps using the materials selection approach outlined in [24].

Fig. 2.1 gives the idea of materials selection for light and stiff compounds. The guide lines in this figure indicates

- E/ρ =C (minimum weight design of stiff ties; minimum deflection in centrifugal loading, etc.)
- $E^{1/2}/\rho$ =C (minimum weight design of stiff beams, shafts and columns)
- $E^{1/3}/\rho$= C (minimum weight design of stiff plates)

The property ranges are also useful in property checking of the new data. When creating a database and to tabulate the new data, property ranges are useful in checking whether each new data lies within the given property ranges.All properties have well defined ranges and new data should generally lie in its proper band.Any discrepancy may then easily be checked again so as to avoid any gross errors from occurring in the compilation.
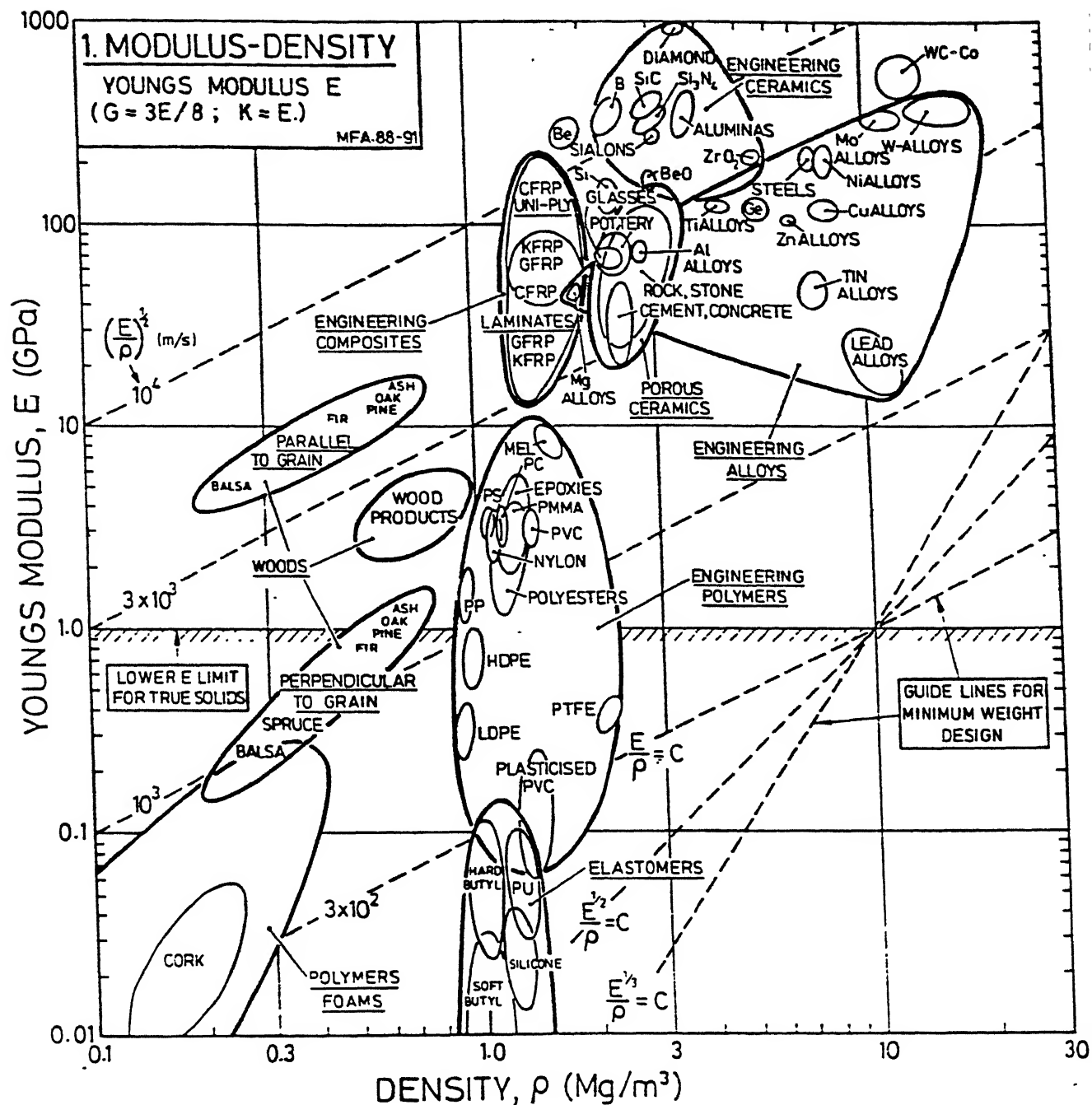
Fig. 2.1 : Materials selection chart between young's modulus E and density ρ

Table2.2:Property (Physical) ranges for various categories of materials

Property	Material					
	Metals	Ceramics	Polymers	Composites	Intermetallics	Refractory * compounds
Physical properties						
Density, gm/cc	0.5-23	1-15	0.75-5	0.3-15	2-20	2-17
Melting point,K	234-3700	140-4000	200-800	250-1750	500-3000	400-4840
Electrical conductivity,1/Ωcm	10^5-10^9	10^{-19}-10^{-5}	10^{-16}-10^{-9}	-	10^3-10^9	10^{-12}-10^{-5}
Thermal conductivity,W/m/K	5-500	1-500	0.01-10	0.1-2	0.2-75	0.2-70 (at 300K)
Coefficient of linear thermal expansion, K^{-1} (x10^{-6})	5-50	1-20	20-300	2-50	1.15-184.3 (at 300K)	0.129-11 (at 300K)
Heat of formation, k.cal/mole	-	-	-	-	1-200	100-272
Cohesive energy 10^5 (J/m)	-	-	-	-	-	2-15

(* Binary borides, carbides, nitrides and oxides ceramic compounds)

2:Property (Mecahnical) ranges for various categories of materials(continued)

Property	Material					
	Metals	Ceramics	Polymers	Composites	Intermetallics	Refractory * compounds
modulus,GPa	1.7-100	7-1000	0.001-20	0.5-700	50-500	40-675
nodulus,GPa	1-200	-	-	-	20-250	75-200
odulus,GPa	25-400	-	-	-	50-300	95-245
n's ratio	0.1-0.5	-	-	-	0.1-0.5	0-.32
e toughness,MPam$^{1/2}$	5-50	0.1-10	0.5-5	1-60	1-50	1-55
temperature, K	5-200	-20-2000	0-200	0-2000	200-1500	150-1600
gation	-	-	-	-	0-50	0-20
constant(C_{11}), GPa	-	-	-	-	50-500	200-500
strength, MPa	10-2000	3000-50000	0.2-400	2.5-1000	100-1500	140-300
strength, MPa	50-2000	1-800	5-100	100-1000	200-1500	65-150
ardness, GPa	-	-	-	-	1-20	410-3370

2.5 Property Ranges for Ceramic Compounds

Property range data for metals, polymers, ceramics and composites have been reported by [23]. In this section we are presenting data on property ranges for refractory compounds based on a data compilation developed by us [20]. The property ranges for various categories of materials are shown in Table 2.2. The structure of data is as follows and typical data sheet is shown for TiC.

Table2 3· Typical data sheet for **TiC** compound

Crystallographic data	Space group	Fm3m	[40]
	Crystal system	cubic(NaCl)	[40]
	Strukturbericht type	O_h^5-F m3m	[40]
	Lattice constant	a=b=c=4.3270	[40]
	Pearson symbol	cF8	[40]
Thermal data	Melting Temperature, T_m(°C)	3065	[44]
	Heat of formation,$-\Delta H_f$(k.cal/mole)	-	
Physical data	Density, ρ(kg/m^3)	4650	[44]
	Electrical resistivity (Ω-m)	10^{-6}	[44]
Mechanical data	Hardness	93 (Vickers)	[43]
	Elastic modulus,E(GPa)	447	[43]
	Shear modulus ,G(GPa)	186	[43]
	Bulk modulus, K(GPa)	241	[43]
	Poisson's ratio,ν	0.19	[43]

*Various nomenclature of crystal structures of binary ceramic compounds are shown in Appendix.

Various data for borides, carbides, nitrides and oxides are shown in Table 2 4-2.7 A comparison between these data and conventional materials is included in Figs.2.2-2.9 . Thus Figs 2.2- 2.9 shows the schematic representation of property ranges for various properties for different categories of materials including borides, carbides, nitrides, and oxides (binary) ceramic compounds. Fig 2.10 summarizes all property ranges of refractory compounds.

Table2.4: Various property data for borides

Boride	Str.	Density (gm/cc)	Melting temp (K)	ΔH (kJ/mole)	$\rho(\Omega cm)$	H (kg/mm^2)	E(GPa)	α (10^{-6}) K^{-1}
Ti$_2$B	Tetra	-	2477	-			3.7	
TiB$_2$	Hexa	4.52	3144	-319.69	26x10^{-6}	3370		6.39
ZrB	Cubic	6.7	-	-318	6x10^{-6}	1560		
HfB	Cubic	12.80	3172	-332				
HfB$_2$	Hexa	11.2	3522	-324	10x10^{-6}	2400		5.3
VB	Ortho	5.4	2522	-136				5
NbB	Ortho	7.6	2533	-		2200		
TaB	Ortho	14.29	2760	-				
TaB$_2$	Hexa	12.6	3366	-206	68x10^{-6}	2537	250	5
CrB	Ortho	6.11	2272	-73.68				
CrB$_2$	Hexa	5.6	2422	-91.37	21x10^{-6}	1700		11.1
MoB	Tetra	8.77	2452	-				
MoB$_2$	Hexa	7.78	2747	-				
W$_2$B	Tetra	16.72	2944	-	21x10^{-6}			4.7
TiB	Cubic	5.26	2333	-159				
WB		15.5	2860			3750		
UB$_2$	Hexa	12.73	2644	-162				
UB$_4$	Tetra	9.38	2755	-244				
UB$_{12}$	Cubic	5.86	2505	-438				
ZrB$_2$	Hexa	6.1	3000		9.2x10^{-6}	2200	350	6.83

le2.5: Various property data for Carbides

npound	T_m K	Dens (gm/cc)	E (GPa)	Shear (GPa)	Bulk (GPa)	ν	K_{IC} MPam$^{1/2}$	K W/mK	$\rho 10^{-3}\Omega m$	ΔH eV
)	2680	2.45	440	186	245	.19	2.6	27	1x10^5	
)	3770	7.6	320	129	197	.22	2	14	70	8.5
	2970	3	390	175	188	.14	3	90	1000	8.7
)	4050	13.4	360	145	220	.22	2	20	25	5.2
)	3440	4.9	420	165	240	.22	2	18	177.8	4.15
)	3000	15.5	600	243	350	.02	2	28	63.1	
)	3300	6.6	346	140	220	.22	2	21	70	5.6
_	-	-	289	165	293	.19	-	-	-	-
C	4203	12.67	179	241	100	.17	-	-	-	5.7
2C	-	-	316	200	268	.10	-	-	-	-
)	2769	13.6	389	157	296	.22	-	-	-	3.7
oC	2866	3	330	197	248	.22	-	-	-	-
)	-	-	241	215	255	.24	-	-	-	3.7

Thermal Cond.

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Table 2.6: Various property data for nitrides

Nitrides	Crystal struct.	Density (gm/cc)	Melting temp.(K)	Young mod. $10^5 Nmm^{-2}$	Micro Hardness $10Nmm^{-2}$	α 10^{-6} K^{-1}	Resis. 10^{-6} Ωcm	K_{IC} $MPam^{1/2}$
AlN	Hex	3.05	2200	3.15	1200	6	10^{11}	60
BN	Hex	2.25	3000	0.9	4400	3.8	10^{14}	
CrN	Fcc	6.1	1050	4	1800	2.3	640	
Cr_2N	Hex	5.9	1725	3.13	1800	9.4		
HfN	Fcc	0.452	3310	3.33	1700	6.9	26	
Mo_2N	Fcc	8.8	700		630			
NbN	Fcc	8.4	2573	4.834	1400	10.1	60	
Nb_2N	Hex	8.3	2430		2120	3.26		
Si_3N_4	Hex	2.8	2160	2.1	1410	2.4	10^{18}	15
TaN	Hcp	14.0	3000	5.76	3240	3.6	128	
Ta_2N	Hex	15.8	3000		3000		263	
TiN	Fcc	5.21	3223	2.5	2450	9.35	25	
UN		14.32	3123			8.1		
VN	Fcc	6.02	2450	4.6	1520	8.1	85	
WN	Hcp				2500			
W_2N	Fcc	12	700				100	
ZrN	Fcc	6.93	3000	5.1	2000	6	13.6	
Be_3N_2		2.7	1866					
Mg_3N_2		2.71	1644					

Table2.7: Various property data for oxides

Oxides	$T_{m=}$(K)	ρ (gm/cc)	Young modulus (GPa)	Shear Modulus (GPa)	Bulk modulus (GPa)	Resistivity (10^{-8} ohm-m)	Heat of fusion kJ/kg	ϑ	K_{IC} MPam$^{1/2}$	α 10^{-6} /K	K W/mK	Hardness 10^3
Al$_2$O$_3$	2320	3.75	330	100	220	-	1060	.26	3.5	8	24	15
?eO	2820	2.8	340	117	315	1×10^{9}	3200	.32	2	7	260	1.1
?gO	3080	3.54	270	92	226	1×10^{20}	1900	.35	2.7	9	30	5
?rO$_2$	2950	5.7	180	60	120	1×10^{17}	760	.2	2	7	2	1.2
?iO$_2$	-	2.15	69	29	38	1×10^{20}	-	.18	.6	.52	1.2	5
?eO	1650	5.7	-	-	-	1×10^{9}	-	.2	.1	-	-	-
?iO	2263	6.67	9.58	3.42	19	1×10^{10}	-	.26	-	-	-	-
?aO	2845	3.34	-	7.37	11	1×10^{12}	-	.20	-	1.29	-	-
nO	2253	5.67	-	-	1.28	1×10^{13}	-	.10	-	-	-	-
?iO$_2$	2103	4.25	-	10	20.7	1×10^{15}	-	.15	-	7.5	-	-
?hO$_2$	3478	10	24	9.32	-	1×10^{19}	-	.20	-	9.4	-	-
?oO	2090	6.4	191	72	183	-	-	.20	-	-	-	-
?O$_2$	3143	10.97	17.2	9.37	47	-	-	.32	-	8.6	-	-

Metal

Low alloy steels
Cobalt alloys
Ti alloys
Lead alloys
Lead alloys

Ceramics

Ice
Diamond
Soda-glass
MgO

Polymers

Nylon
Epoxies
Kelvar

Composites

BFRP
CFRP
GFRP
Woods

Intermetallics

Ti-Al
Al-Fe
Ni-Al

Boride

CrB
FeB
HfB
LaB_6
NbB
TiB_2
WB
ZrB

Carbide

WC
TiC
BC
NbC
TaC
MoC
UC

Nitrides

AlN
CrN
HfN
MoN
UN
VN
WN
TiN
ZrN

Oxides

Al_2O_3
BeO
CaO
CoO
MgO
NiO
ThO_2
UO_2

Density gm/cc

20 15 10 5 0

Fig.2.2: Property ranges for Density for various category of materials
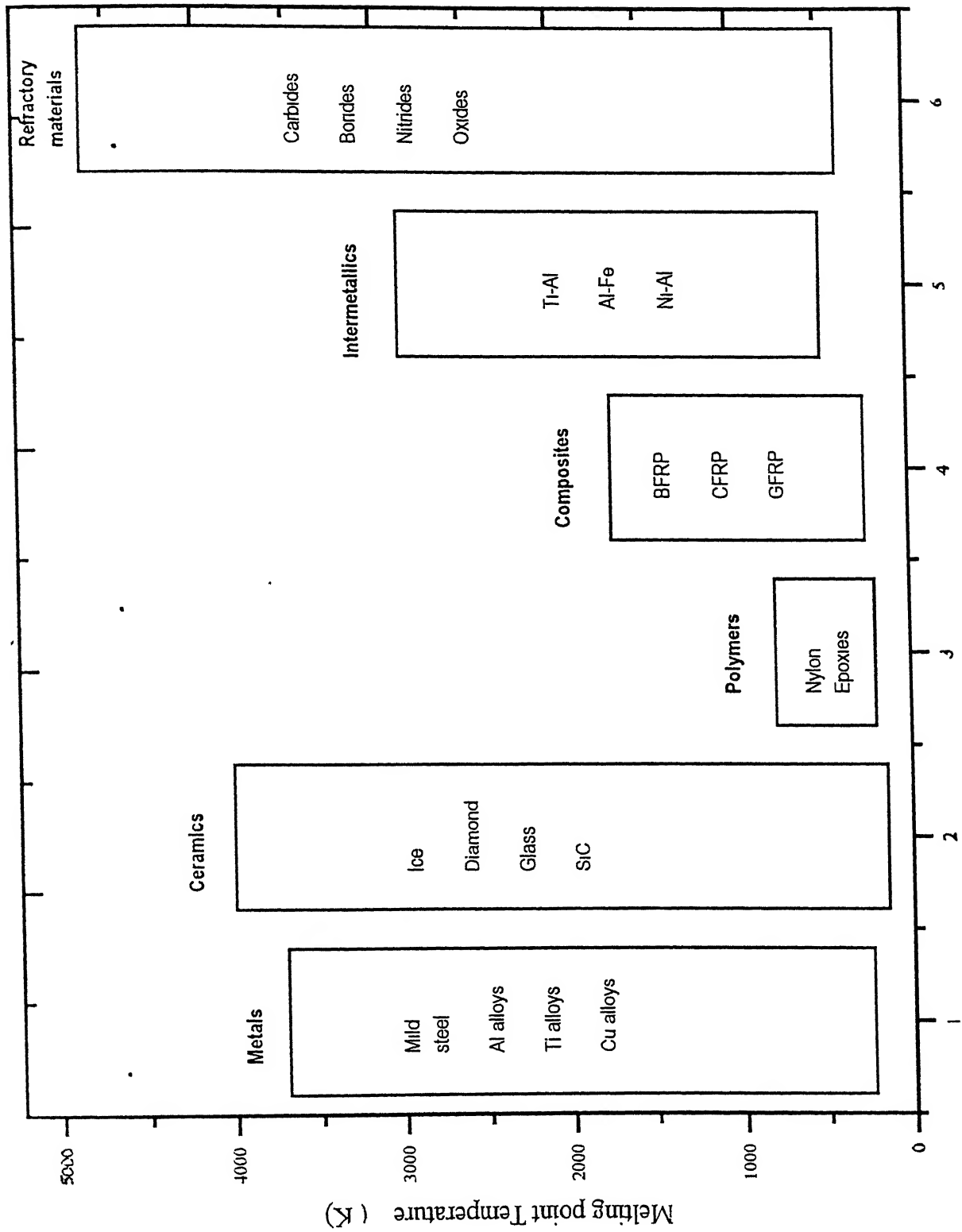
Fig 2.3: Property ranges for melting Temperature for various category of materials

30
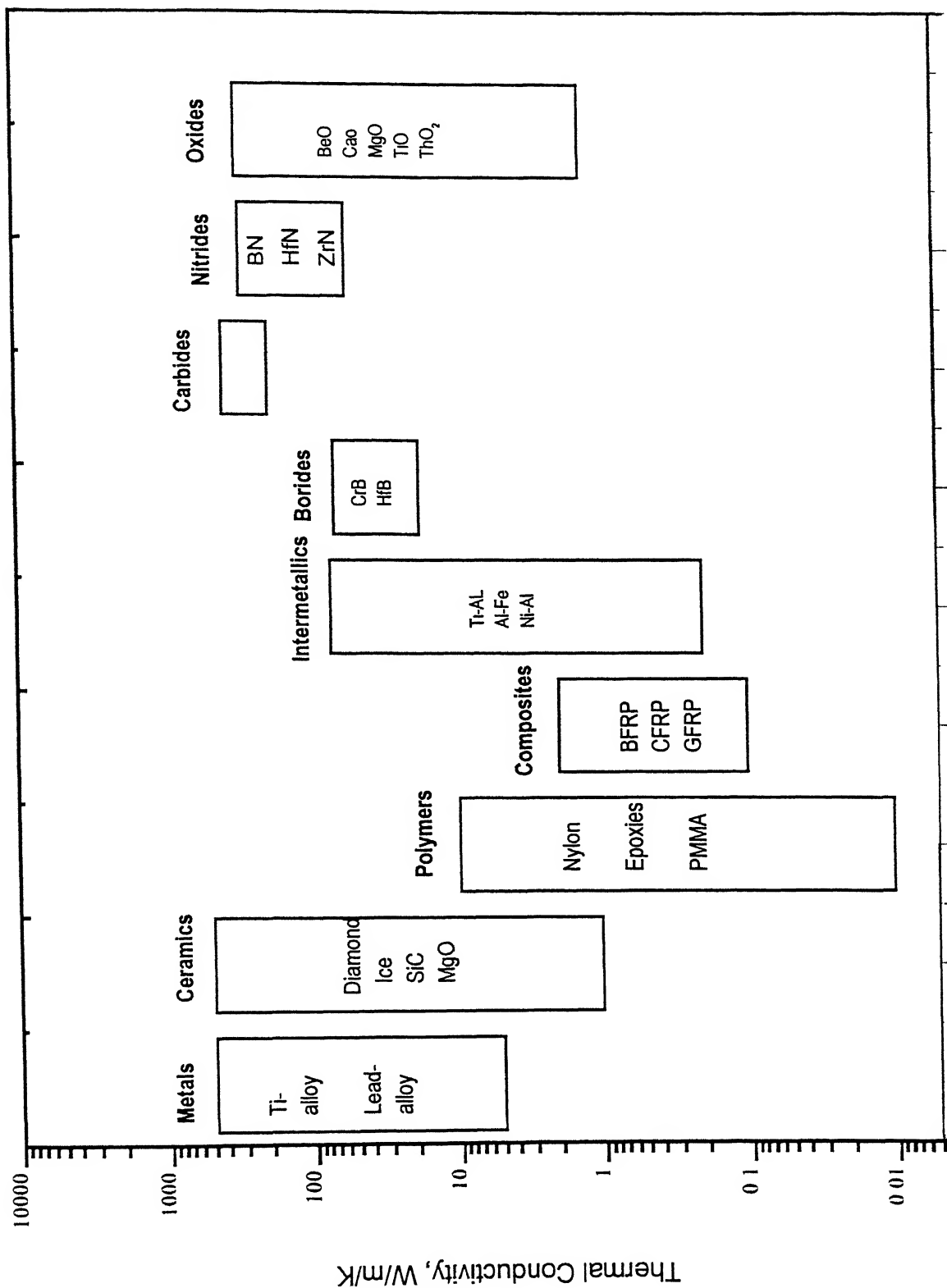
Fig.2.4 Property ranges for Thermal Conductivity for various category of materials
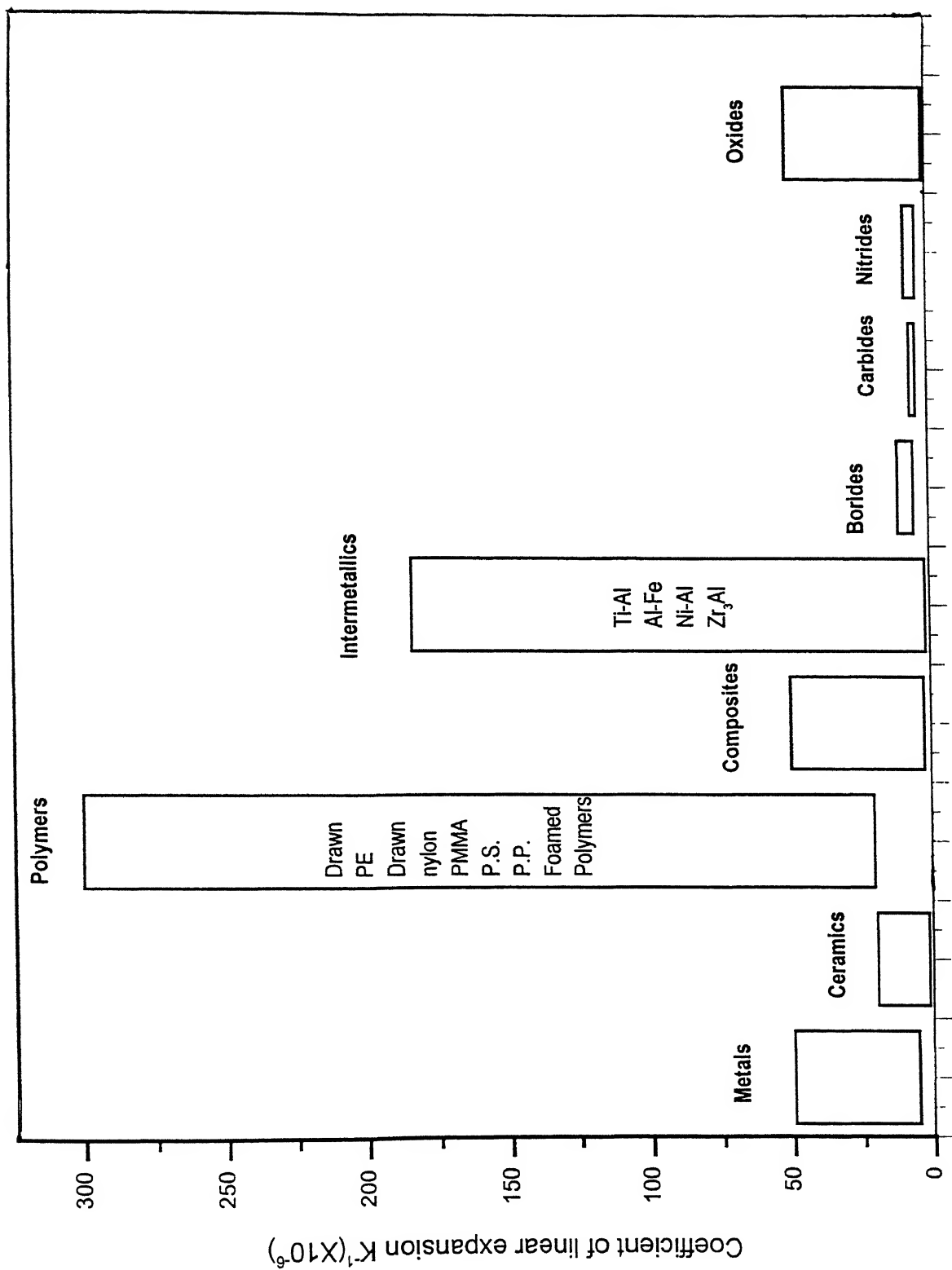
Fig.2.5:Range of coefficient of thermal expansion for various category of materials

Ceramics

Diamond
Ice
MgO
SiC

Metals

Ti-alloys
Lead-alloys
Mild-steel

Polymers

Nylon

Composites

BFRP
CFRP
GFRP

Intermetallics

Ti-Al
Al-Fe
Ni-Al

Carbides

AlC
HfC
BC
NbC

Borides

AlB
HfB
CrB
ZrB

Nitrides

AlN
CrN
HfN
MoN
WN
UN
ZrN

Oxides

BeO
CoO
MgO
ThO

Yield strength Mpa

0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
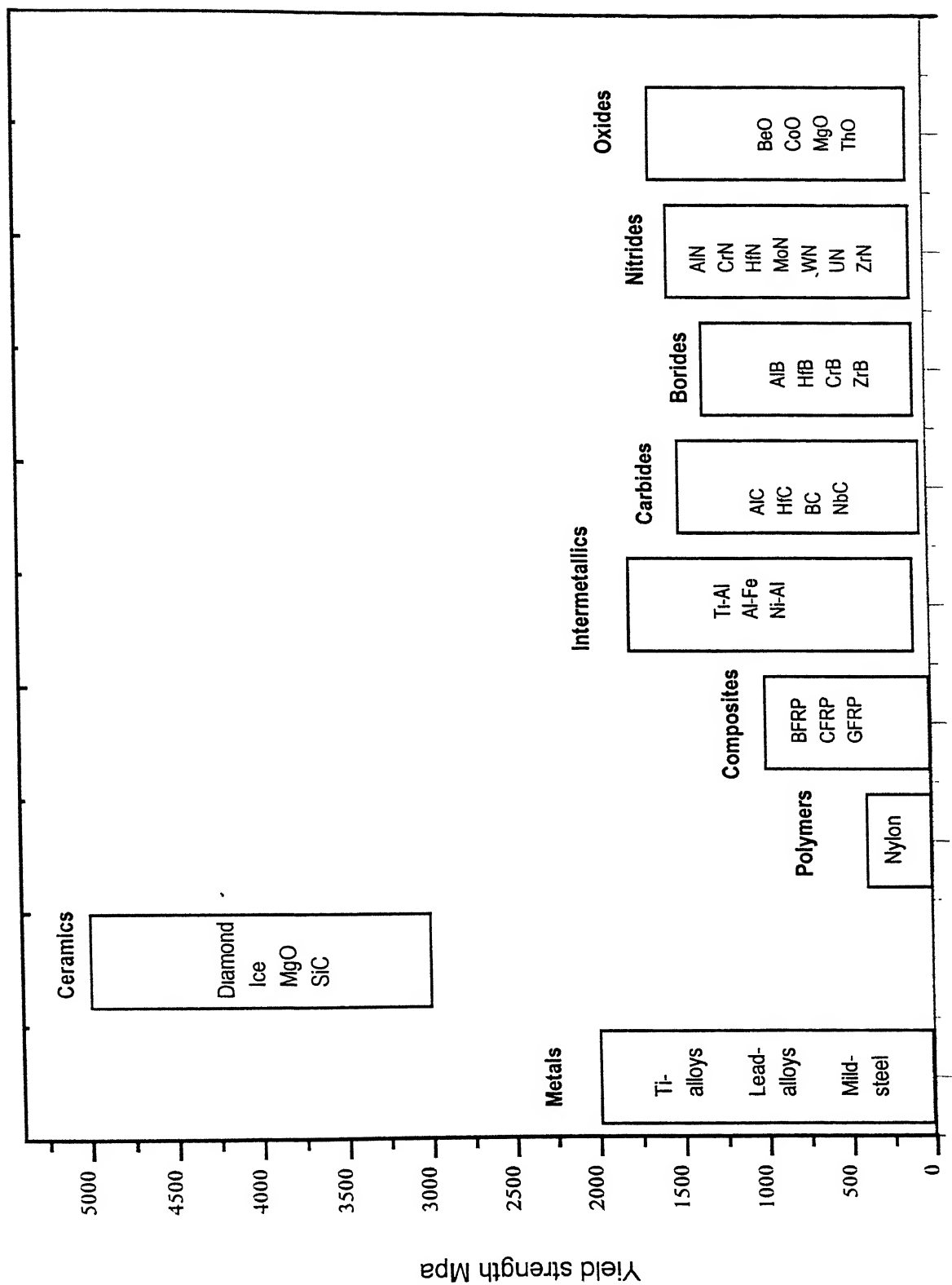
Fig.2.6:Property ranges for yield strength for various category of materials

33
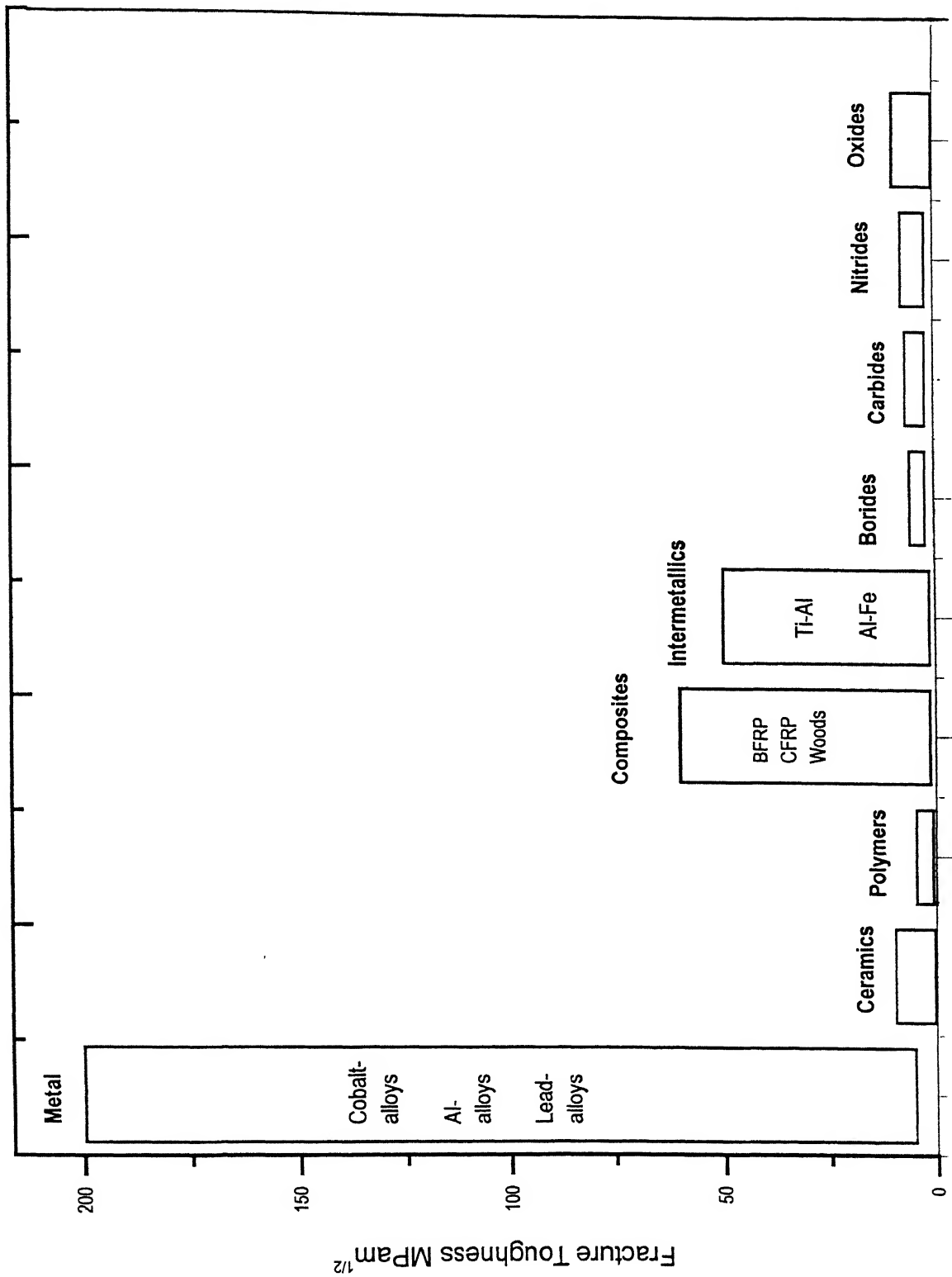
Fig.2.7:Property ranges for various category for Fracture toughness for various category of materials
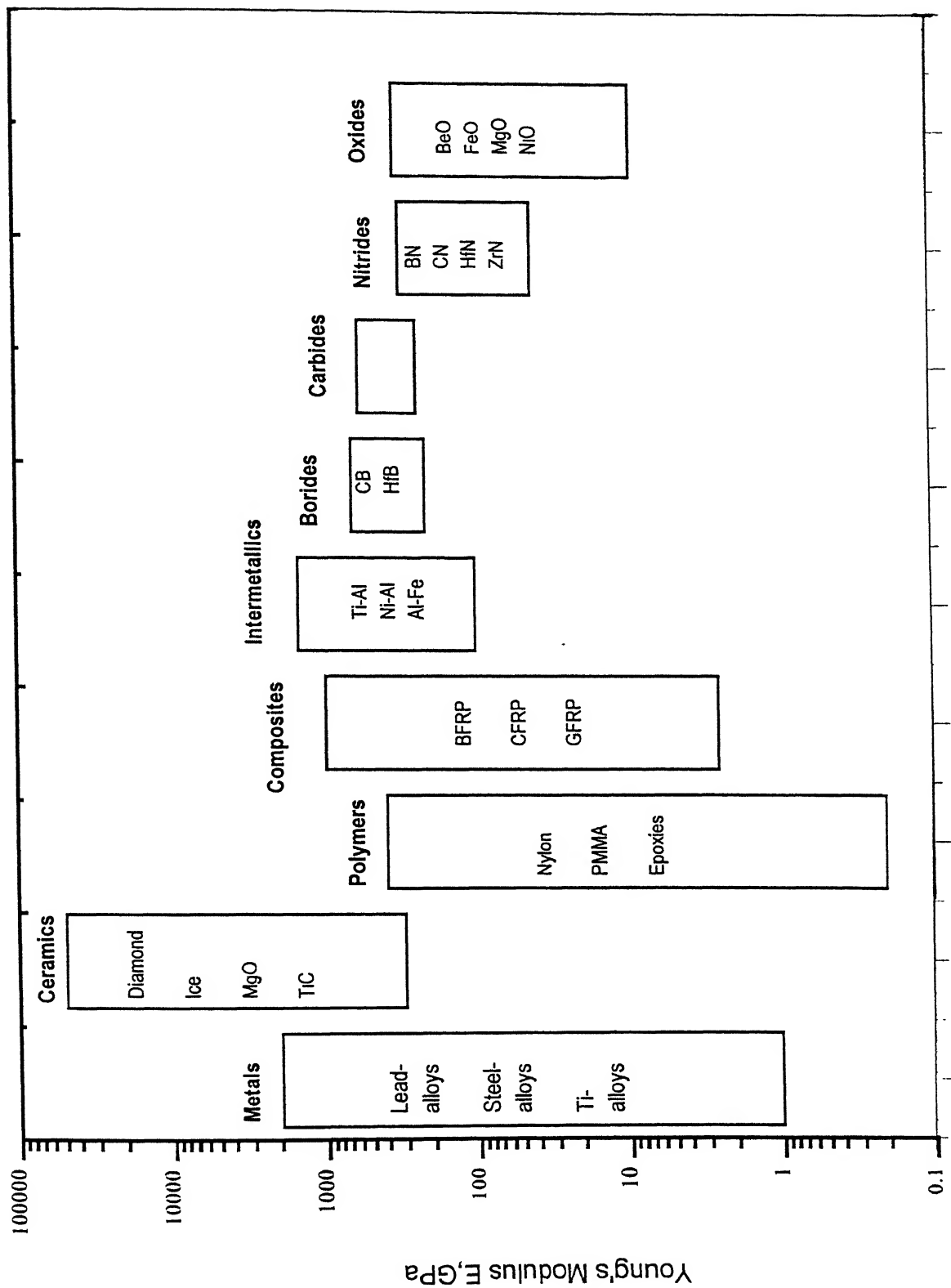
Fig.2.8:Property ranges for elastic modulus (E)for various categories of materials

Young's Modulus E,GPa

Metals
Lead-alloys
Steel-alloys
Ti-alloys

Ceramics
Diamond
Ice
MgO
TiC

Polymers
Nylon
PMMA
Epoxies

Composites
BFRP
CFRP
GFRP

Intermetallics
Ti-Al
Ni-Al
Al-Fe

Borides
CB
HfB

Carbides

Nitrides
BN
CN
HfN
ZrN

Oxides
BeO
FeO
MgO
NiO

100000
10000
1000
100
10
1
0.1
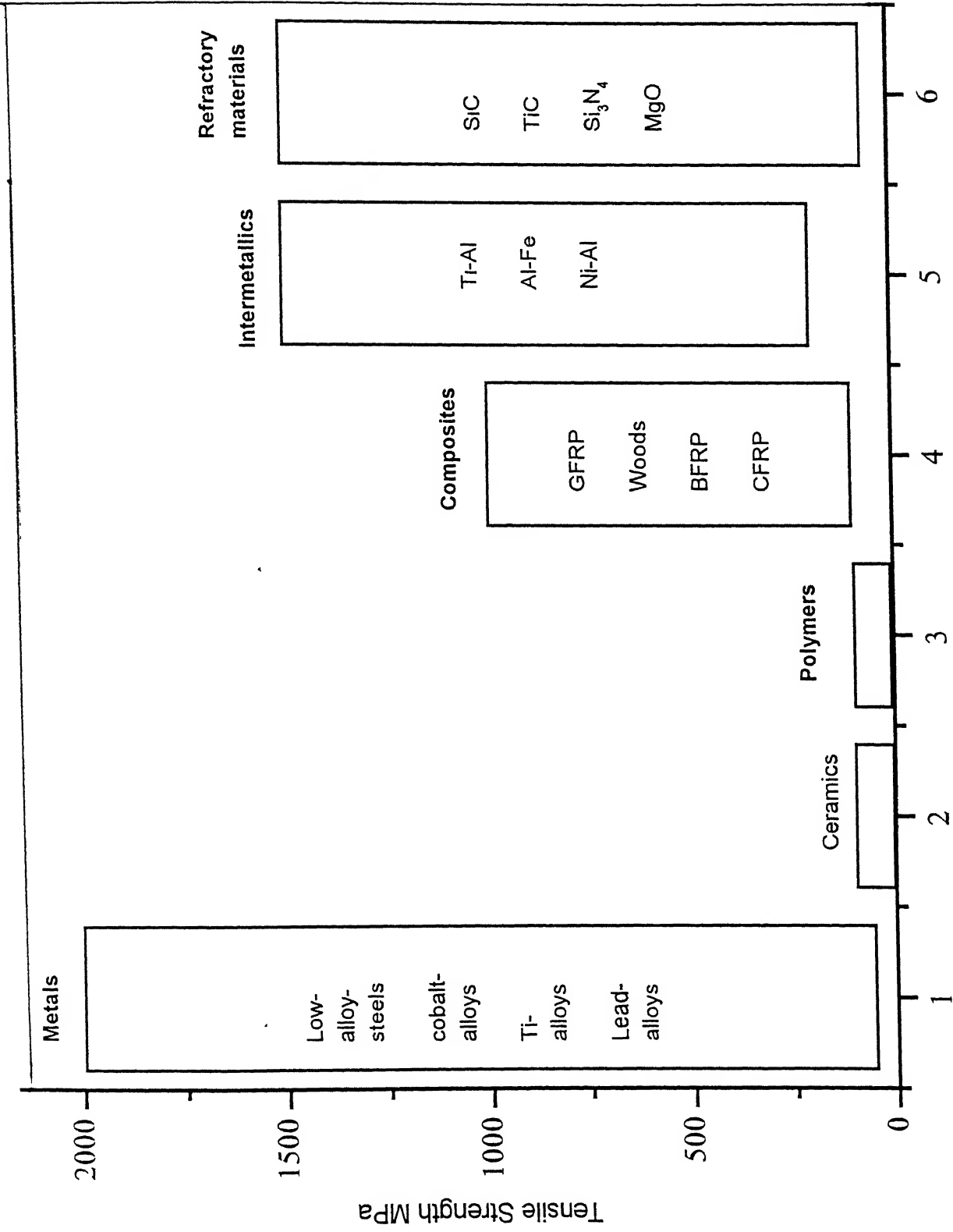
Fig.2.9:Property ranges for Tensile Strength for various category of materials

Density gm/cc

Melting point K

Thermal conductivity W/mk

E(GPa)

G(GPa)

K(GPa)

Poisn. ratio

Fracture toughness MPam$^{1/2}$

Creep temp. K

% elongation

C$_{11}$

Bend strength MPa

Tensile strength MPa

MicroHardness

10000
1000
100
10
1
0 1
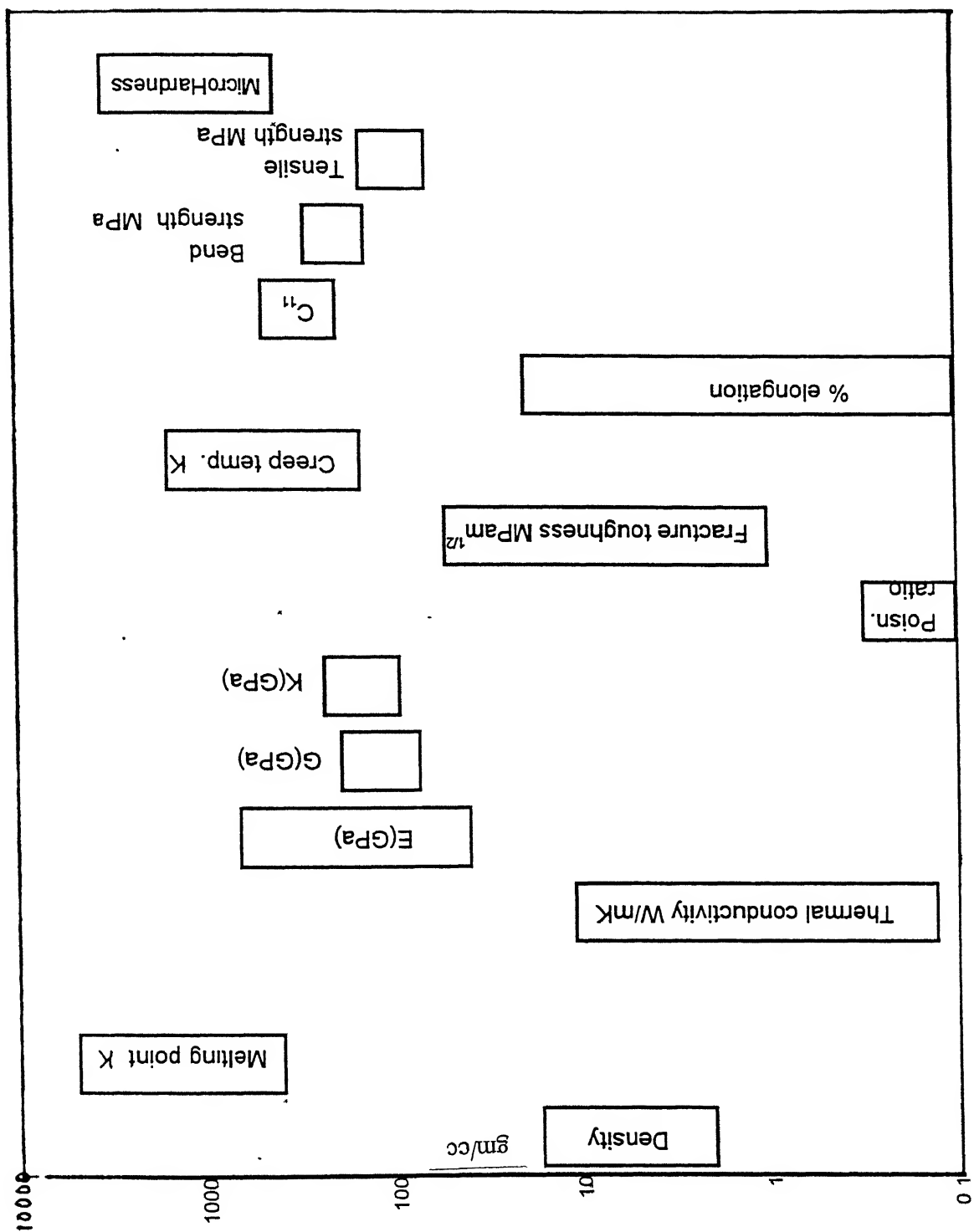
Fig 2 10· Property ranges for various properties of refractory materials

Chapter 3

Correlations in Ceramic Compounds

3.1 Literature Survey

A number of correlations between various physical properties have been investigated over the years for various classes of materials [9,34].Some correlations have a physical basis whereas others are empirical. In this chapter we will investigate the applicability of some of these correlations to refractory compounds. We first review some of the important correlations.

(a) Atomic Volume V_M (m^3/ k.mole)

The atomic volume denoted by V_M is given as

$$V_M = \frac{\overline{A}}{\rho} \tag{3.1}$$

Where $\overline{A}$ is average atomic weight of the compound in (kg/k.mole) and the density ρ in Kg/m^3. The average atomic weight of the compound is given by

$$\overline{A} = \frac{mA_X + nA_Y}{m+n}$$

where A_X and A_Y are the atomic weights of X and Y respectively.

(b) Relation between Elastic modulus E, Shear modulus G, Bulk modulus and Poission's ratio ν

We know for isotropic materials

$$G = \frac{E}{2(1+\nu)} \qquad (3.2)$$

$$K = \frac{E}{3(1-2\nu)} \qquad (3.3)$$

Theoretically ν may range between -1 and 0.5. However, for most materials ν varies between 0.2 and 0.4. We can therefore write above two relations as

$$C_L < \frac{G}{E} < C_H \qquad (3.4)$$

$$C_L < \frac{K}{E} < C_H \qquad (3.5)$$

where C_L and C_H are lower and upper limits of the correlation based on the actual compiled data.

(c) Relation between Elastic modulus E (GPa), Melting temperature T_m(K)

(i)   Relation between Elastic modulus E (GPa), Melting temperature T_m(K), Atomic Volume V_M (m^3 / k.mole) and Gas constant R (kJ/k.mole.K)

If the bonds between the atoms are stretched too far, they break. Similarly heat can break the bonds and results in melting or sublimation. This is the basic relationship between elastic modulus and melting temperature . Bond stretching is characterized by bulk modulus K. The thermal energy per atom or molecule at melting point is RT_m/k.mole.

$$\frac{KV_m}{RT_m} = \text{constant}$$

Where R is the gas constant (8.314 kJ/k.mole.K).Expressing the above correlation with upper and lower limits,

$$C_L < \frac{KV_m}{RT_m} < C_H$$

$$C_L < \frac{EV_m}{RT_m} < C_H \qquad (3.6)$$

Similar relation can be obtained for E, V_m, T_m and C_P (KJ/Kmole.K) and is given by

$$C_L < \frac{EV_m}{C_p T_m} < C_H \qquad (3.7)$$

(ii)   Relation between Elastic modulus E(GPa), Melting temperature T_m (K),Density ρ (Kg/m^3) and Specific heat C_P(kJ/kg.K)

The heat capacity is the heat required to raise the temperature of a solid by 1K. The molar heat capacity $C_v{}^m$ (J/k.mole.K) is given by

$$C_v{}^m \approx 3R$$

$$C_V (kJ / kg.K) = \frac{3R}{\rho V_m}$$

In solid state heat capacity at constant pressure C_P is equal to that at constant volume, giving correlation

$$C_L < \frac{C_P \rho V_m}{R} < C_H \qquad (3.8)$$

From equation 3.6 and 3.8, eliminating $\dfrac{V_m}{R}$, then eq. 3.8 becomes,

$$C_L < \frac{C_P \rho T_m}{E} < C_H \qquad (3.9)$$

(d) Relation between Microhardness H (GPa), Melting temperature T_m(K),Atomic volume V_m (m^3/k.mole), Boltzmann constant k (J/K) and Avagadro number(N)

The   plot between microhardness and melting points shows that microhardness increases with melting temperature in Fig. 3.1. This shows that hardness and melting temperature are not independent variables. Low melting materials tend to be soft and high melting materials are hard. So we can say that microhardness varies linearly with melting temperature.

$$H \propto T_m$$

$$HV_m \propto Nk T_m \quad \text{Where } k=1.38 \times 10^{-23} \text{ J/K, } N=6.02 \times 10^{26} \text{ /kmole}$$

$$\frac{HV_m}{NkT_m} = \text{constant}$$

therefore
$$C_L < \frac{HV_m}{NkT_m} < C_H \qquad (3.10)$$

similar relation can be obtained by replacing Nk with C_P (kJ/k mole.K) as

$$C_L < \frac{HV_m}{C_P T_m} < C_H \qquad (3.11)$$

(e) Relation between Specific heat C_p (kJ/kg.mole), Density ρ (Kg/m^3), Melting temperature T_m (K) and Hardness H (GPa)

From eq. 3.9, materials with higher elastic modulus will be having higher melting point and so hardness also. So we can write eq.3.9 as

$$C_L < \frac{C_P \rho T_m}{H} < C_H \qquad (3.12)$$

or from eq 3 10, using Nk=R (Gas constant)

$$C_L < \frac{HV_m}{T_m R} < C_H \qquad (3.14)$$

Some examples of values for limits of correlations for metals and alloys, ceramics, polymers and elastomers are shown in table 3.1

Table 3.1: Examples of values for limits for correlations [8]

Material class	Metals and Alloys		Ceramics		Polymers		Elastomers	
Property Group	C_L	C_H	C_L	C_H	C_L	C_H	C_L	C_H
G/E	0.3	0.4	0.33	0.5	0.29	0.41	0.3	0.5
K/E	0.5	2.0	0.55	2.2	1.0	3	20	1000
KV_m/RT_m	60	150	48	120	1.9	16	5.6	10
EV_m/RT_m	80	180	70	120	0.5	16	5.6	10
$C_p\rho V_m/R$	1.4	4.9	2.5	5.2	1	2.4	1.4	3.5
$C_p\rho T_m/K$	0.02	0.05	0.022	0.05	0.08	0.6	0.2	0.4
$K\alpha/C_p\rho$	0.3	0.84	0.25	0.9	0.05	0.24	0.14	0.25
$\alpha T_m(x10^{-3})$	14	27	4	28	18	60	19	180
$\lambda/bC_p(E\rho)^{1/2}$	$1.5x10^6$	$2.4x10^7$	$4x10^5$	$5x10^6$	$2.5x10^4$	$8x10^5$	$1.5x10^6$	$1.5x10^7$
$L_m\rho V_m/RT_m$	0.9	1.2	0.8	1.3	NA	NA	NA	NA
L_m/C_pT_m	0.24	0.47	0.5	0.9	NA	NA	NA	NA
$L_m\rho/K$	0.008	0.022	0.015	0.38	NA	NA	NA	NA
T_g/T_m	0.5	0.6	0.5	0.6	0.6	0.75	NA	NA
σ_y/E	0.2	8	10	40	6	60	1000	8000
σ_{ts}/σ_y	1.1	2.5	1.0	1.2	1.1	2.0	1	1.1
σ_{ts}/E	1.2	7.0	0.1	36	8	95	1000	8000
σ_{MOR}/σ_y	1.05	1.2	1.05	14	1.1	1.6	1	1.2
σ_c/σ_y	1	1.2	8	18	1.2	1.5	1	4
H/σ_y	2.2	7.5	3	200	2.8	4	3	10
σ_e/σ_{ts}	0.23	1.3	0.8	1	0.35	0.9	0 3	1
$K_{IC}/\sigma_y\sqrt{b}$	2000	36000	6	170	150	6500	0.1	150
G_C/Eb	16	2500	0.05	4	25	$3x10^5$	0.1	$2x10^5$
$K_{IC}/E\sqrt{b}$	4	50	0.2	2	3	18	0.3	450

(f) Correlation between Elastic modulus E, Density ρ, coefficient of thermal expansion α and specific heat C_p

The correlation between elastic modulus E, density ρ, coefficient of thermal expansion α and specific heat C_p is given by [8].

$$C_L < \frac{E\alpha}{C_P\rho} < C_H \qquad (3.15)$$

3.2 Results and Discussions

In this section, we present results for correlation described in section 3.1. Section 3.2.1 discuss the relations between E,G and K for some of the refractory compounds section as a case study for carbides, borides, nitrides and oxides.

3.2.1 Correlations for Refractory compounds of Oxides and Carbides

As seen in the preceding section, better correlations and estimates are expected based on individual classes of materials. Therefore, correlations have been developed for various classes instead of the entire range of refractory compounds. Typical results for borides, carbides, nitrides and oxides are presented in Table 3.2 -3.5

Table 3.2: Different values for Borides

Property relation (equation number)	Units	C_L	C_H
$\dfrac{EV_m}{RT_m}$	E in Gpa V_m in m^3/k.mole R in kJ/k.mole.K	20.0	116
$\dfrac{EV_m}{C_P T_m}$	C_p in kJ/kg.K	0.10	1.91
$\dfrac{C_P \rho V_m}{R}$	C_P in kJ/kg.K ρ in kg/m^3	0.054	9.67
$\dfrac{C_P \rho T_m}{E}$	H in Gpa k is 1.38×10^{-23} J/K N is 6.023×10^{-23}/k.mole	0.21 .	1.2
$\dfrac{HV_m}{C_P T_m}$	C_P in kJ/k.mole.K	69	165
$\dfrac{C_P \rho T_m}{H}$	C_P in kJ/ k.mole.K	0.4	1.0
$\dfrac{E\alpha}{C_P \rho}$	C_P in kJ/k.mole.K	2.6×10^3	6.8×10^3
αT_m	α in $\times 10^{-6}$/K T_m in K	7.2×10^{-3}	33.7×10^{-3}

Table 3.3 : Different values for Carbides.

Property relation (equation number)	Units	C_L	C_H
$\dfrac{EV_m}{RT_m}$	E in Gpa V_m in m^3/k.mole R in kJ/k.mole.K	12.8	116
$\dfrac{EV_m}{C_PT_m}$	C_p in kJ/kg.K	0.66	1.21
$\dfrac{C_P\rho V_m}{R}$	C_P in kJ/kg.K ρ in kg/m^3	0.75	10.3
$\dfrac{C_P\rho T_m}{E}$	H in Gpa k is 1.38×10^{-23} J/K N is 6.023×10^{-23} /k.mole	0.58	8.8
$\dfrac{HV_m}{C_PT_m}$	C_P in kJ.k.mole.K	48	62
$\dfrac{C_P\rho T_m}{H}$	C_P in kJ/ k.mole.K	0.8	1.7
$\dfrac{E\alpha}{C_P\rho}$	C_P in kJ/k.mole.K	1.5×10^4	15.8×10^4
αT_m	α in $\times10^{-6}$ /K T_m in K	9.35×10^{-3}	27.3×10^{-3}

Table 3.4: Different values for Nitrides

Property relation (equation number)	Units	C_L	C_H
$\dfrac{EV_m}{RT_m}$	E in Gpa V_m in m^3/k.mole R in kJ/k.mole.K	32.8	64
$\dfrac{KV_m}{RT_m}$	K in Gpa	43	61
$\dfrac{C_P\rho V_m}{R}$	C_P in kJ/kg.K ρ in kg/m^3	0.013	0.091
$\dfrac{C_P\rho T_m}{E}$	H in Gpa k is 1.38×10^{-23} J/K N is 6.023×10^{-23} /k.mole	0.04	0.141
$\dfrac{HV_m}{C_P T_m}$	C_P in kJ/k.mole.K	10	39
$\dfrac{C_P\rho T_m}{H}$	C_P in kJ/ k.mole.K	0.14	2.46
$\dfrac{E\alpha}{C_P\rho}$	C_P in kJ/k.mole.K	6.9×10^4	209.8×10^4
αT_m	α in $\times 10^{-6}$ /K T_m in K	2.7×10^{-3}	29.6×10^{-3}

Table 3.5: Different values for Oxides.

Property relation (equation number)	Units	C_L	C_H
$\dfrac{EV_m}{RT_m}$	E in Gpa V_m in m^3/k.mole R in kJ/k.mole.K	2.8	235.2
$\dfrac{EV_m}{C_P T_m}$	C_p in kJ/kg.K	0.052	1.9
$\dfrac{C_P \rho V_m}{R}$	C_P in kJ/kg.K ρ in kg/m^3	0.5	26.9
$\dfrac{C_P \rho T_m}{E}$	H in Gpa k is 1.38×10^{-23} J/K N is 6.023×10^{-23} /k.mole	0.17	0.114
$\dfrac{HV_m}{C_P T_m}$	C_P in kJ/k.mole.K	28	84
$\dfrac{C_P \rho T_m}{H}$	C_P in kJ/k.mole.K	0.3	2.5
$\dfrac{E\alpha}{C_P \rho}$	C_P in kJ/k.mole.K	4.8×10^4	39.1×10^4
αT_m	α in $\times 10^{-6}$ /K T_m in K	0.85×10^{-3}	44.8×10^{-3}

3.2.2 Calculations based on property ranges

As seen in the preceding section, better correlations and estimates are expected based on individual classes of materials . Therefore correlations have been developed for various classes instead of the entire range of binary ceramic compounds.

(a) Coefficient of linear thermal expansion verses melting temperature

Fig 3.1 shows the variation of coefficient of linear thermal expansion verses melting temperature. It can be shown from figure that the distribution follows the relation

$$\alpha \, T_m = \text{constant}$$

where constant is approximately equal to 17752.7 fig. 3 1. This relationship is useful in estimating the unknown properties of either α or T_m is known. This can be expressed as follows.

$$C_L < \alpha T_m < C_H \tag{3.16}$$

Where $C_L = 9.35 \times 10^{-3}$ and $C_H = 27.3 \times 10^{-3}$. Some estimates based on this correlation are shown in Table3.6

Table3.6: Some estimation of α for carbides using the correlation given by eq.(3.16)

Name of the compound	Temperature (K)	Correlation $C_L < \alpha < C_H$	Calculated $\overline{\alpha} \times 10^{-6} \, K^{-1}$	Actual $\alpha \times 10^{-6} \, K^{-1}$	% error
WC	3000	$3.1 \times 10^{-6} < \alpha < 9.1 \times 10^{-6}$	6.1	5.0	22%
ZrC	3300	$2.83 \times 10^{-6} < \alpha < 8 \, 27 \times 10^{-6}$	5.55	6.0	9%

(b) Shear modulus verses Young modulus

Figure 3.2 shows the variation of shear modulus verses young modulus. It can be shown that the distribution follows the relation

$$\frac{G}{E} = \text{constant} \tag{3.17}$$

where constant is approximately equal to 0.42115 from figure 3.2 This relationship is useful in estimating the unknown properties of either G or E. this can be expressed as follows

$$C_L < G/E < C_H \qquad (3.16)$$

Where $C_L = 0.4031$ and $C_H = 0.405$ Some estimates based on this correlation are shown in

Table3.7: Some estimation of shear modulus using the correlation given by eq.3.17

Name of the compound	E (GPa)	Correlation $C_L < G < C_H$	Calculated $\overline{G}$ (GPa)	Actual G (GPa)	% error
WC	600	241.86<G<242	241 93	242	0 02%
ZrC	346	139.47<G<140.13	139.80	140	0.14%

The same treatment can be dealt with nitrides and oxides using the relationships given in table 3.4 & 3.5. These correlations are used in Informed Neural Network dealt in section 5.4.[49]

Carbides

$\alpha T_m = 17752.7$

Melting temperature K

Coefficient of thermal expansion×10⁶K⁻¹

Carbides

Y=0.42115*X

E 10⁶N mm⁻²

G 10⁵N mm⁻²

Nitride

Y=11261.999/X

Melting temperature ˙K.

Coefficient of linear thermal expansion (10⁻¹k⁻¹)

$Y = 11261.999/X$

Coefficient of linear thermal expansion ($10^{-1}k^{-1}$)

Figure showing Linear thermal expansion ($10^{-6}K^{-1}$) versus Melting temperature (°K) for Oxides. Equation: Y=17801.47X

Oxide

Y=.33494X

Shear modulus G (Gpa)

120 100 80 60 40 20 0

Youngs modulus E Gpa

0 50 100 150 200 250 300 350

54

Chapter 4

Correlations based on Mendeleev Number

4.1 Introduction

The description of Mendeleev number is given in chapter 1. The success of Mendelev number in achieving the structural separation for various refractory compounds suggests that Mendeleev number may correlate also with formation and properties Of these compounds. For example the ease of joining two materials (elements) by friction welding varies from good weld formation to no joining. When such information for various materials is described on a chart where the corresponding Mendeleev number of the two materials are plotted on x and y axis, as shown in Fig.4.1 clear separation of material pairs which weld with varying degree of success is obtained [17]. Therefore in this chapter we explore the existence of such correlations between Mendeleev number and some physical properties like density, melting temperature heat of formation etc. Some correlations between two physical properties have already been presented in chapter 3. The approach is adhoc at this stage, but the results may guide us in conducting more systematic studies.
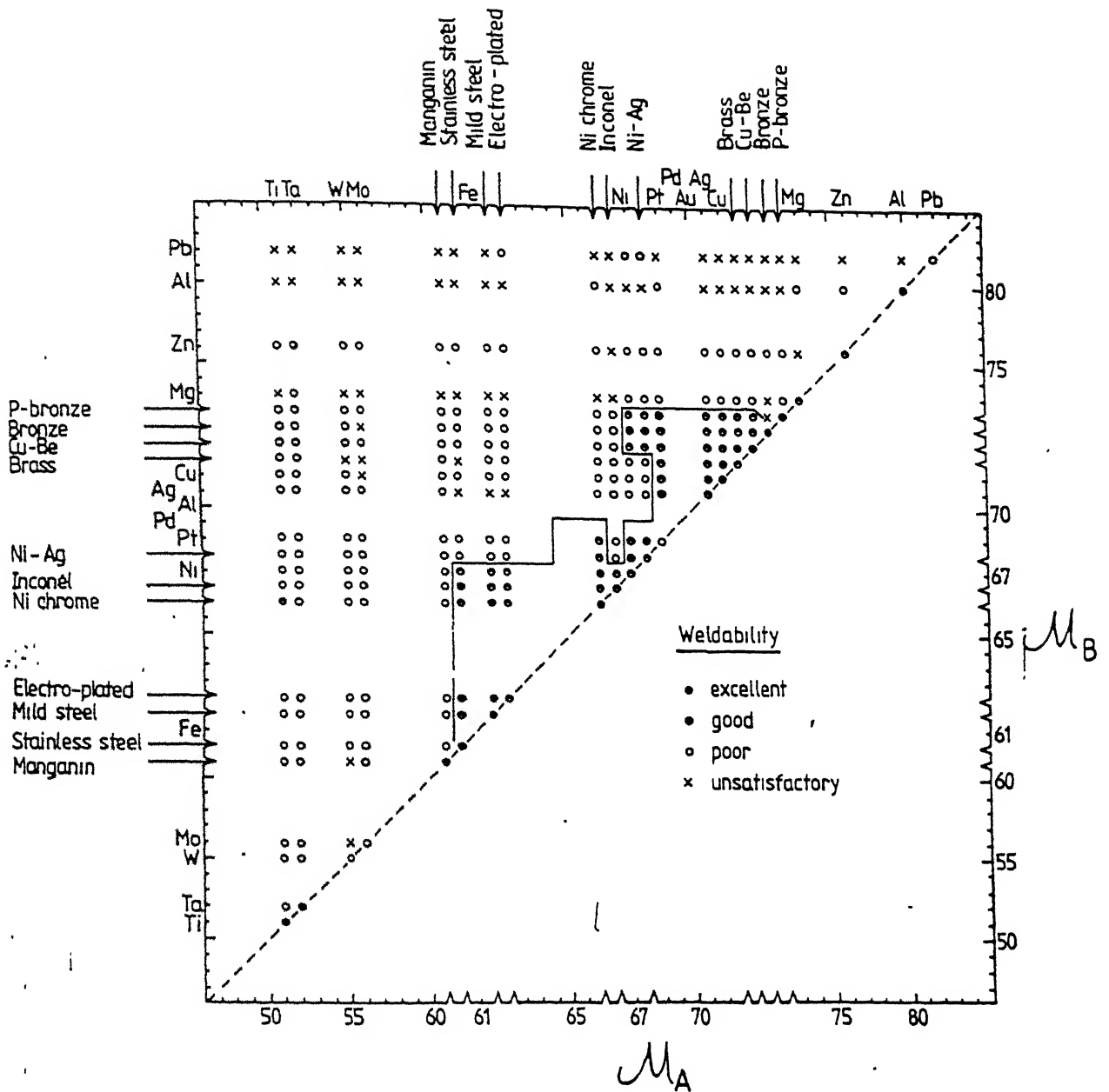
Fig. 4.1: Weldability property chart

4.2 Some Applications of Mendeleev number

For compound, we define an effective Mendeleev number as weighted average of individual Mendeleev numbers of the constituent elements. Similar definition has been used for design of ternary alloys [17]. Some of the important applications of Mendeleev number are

- Study of binary ceramic compounds thermally
- Phase diagram study of ceramic compounds

Now we will look these applications in the detail.

(a) Thermal study of binary Compounds

Using the informations given in [40], on thermal study of binary refractory compounds, we analyzed data in terms of variation with Mendeleev number M. This is shown in Fig. 4.2 and we can observe the three most significant regions of absence of chemical combination ,chemical combination and no thermal study. From Fig 4 2,we can observe that similar types of symbols are grouping together and as the thermal study continues we could see clear separation of these regions well.

(b) Phase diagram study of binary Compounds

Attempts for the existence or non-existence of binary ceramic compounds by phase diagram studies have been made for many years and the data has been compiled in various ways shown in [41]. The data is plotted in terms of Mendeleev number in Fig 4 3 The plot shows a part of chemical element verses chemical element where Mendeleev number is considered for each element. The plot shows clear separation of different regions with same identification. The various types of regions and their corresponding symbols are explained in Fig.4 3
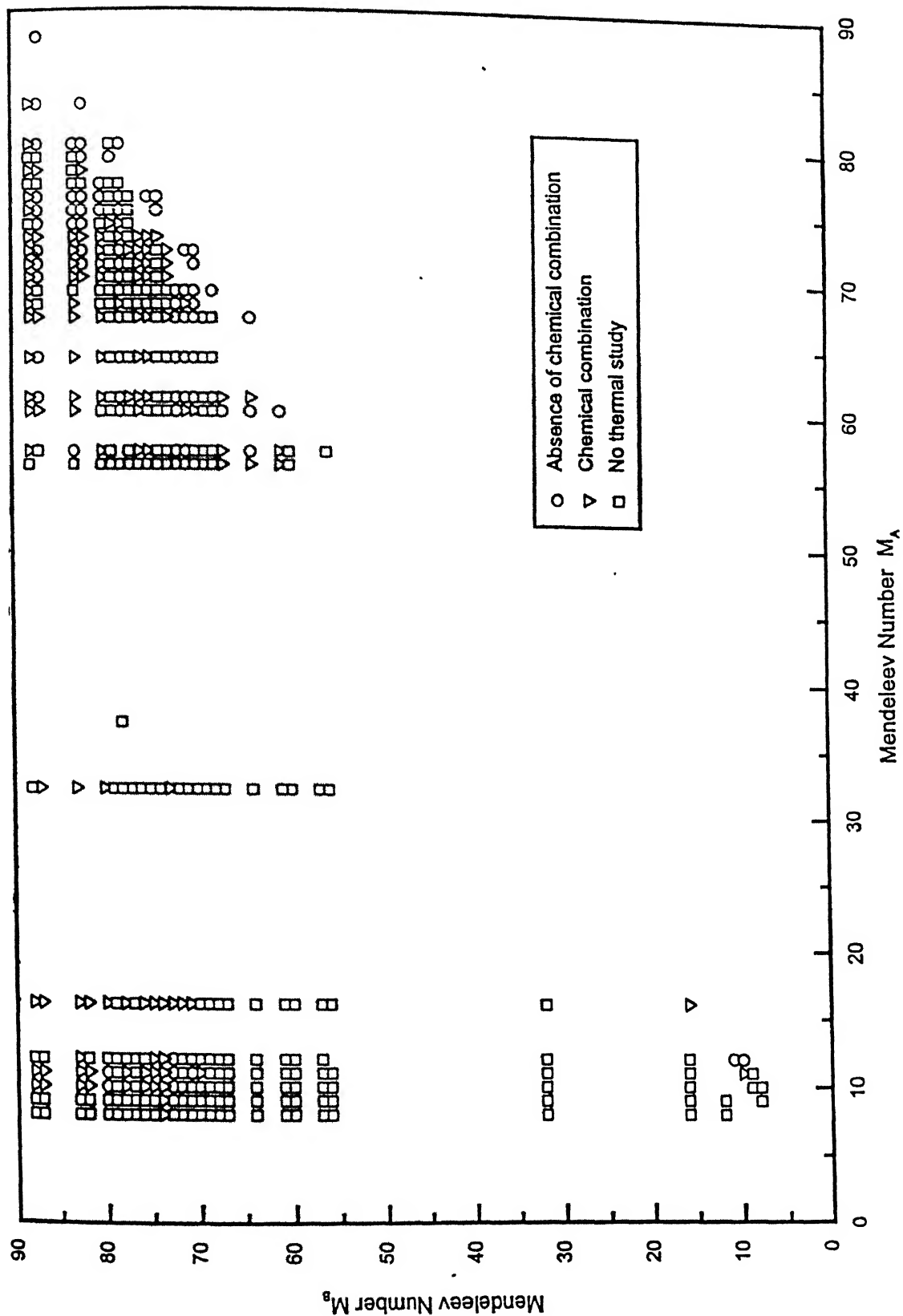
Fig 4.2.: Thermal study of binary ceramic compounds

4.3 Estimation of unknown Density and Melting Temperature of Refractory Compounds

In this section we will study some methods to estimate the unknown values of density and melting temperatures of some Borides, Oxides and Nitrides by studying the variation of Mendeleev number with density as well as melting temperature

4.3.1 Density verses Mendeleev number of binary ceramic compounds

Fig. 4.5 shows the distribution of density of oxides as a function of their average Mendeleev number M_A and density ρ of oxides has been taken from [38] . In Fig 4 7 we see some systematic (linear) patterns appearing in terms of position of groups of compounds: (W, Mo ,Cr)B, (W, Mo, Cr)B$_2$, (*, W, Mo)$_2$ B$_5$, and (Mo, *, Cr)B$_2$ Each straight line represents borides of particular type. These missing compounds, which are denoted by '*' are Cr$_2$B$_5$, WB$_2$ respectively. We can also observe that all of these lines have similar slope. The density of unknown compound can be found by making use of geometrical similarity of these patterns. This requires first the calculation of the average Mendeleev numbers of unknown compounds Using this approach the density values for some of missing compounds are shown in Table 4.1.

Table 4.1: Calculated density values of boride ,nitrides, oxides

Name of the compound	Measured Density (kg/m^3)	Literature Value (kg/m^3)
Cr$_2$B$_5$	11.5	*
WB$_2$	10.5	*
ZrB$_2$	10.2	*
TaO	8.23	*
RaO	6.6	*
TaN	14.0	14.36
Mo$_2$N	8.8	8.04
V$_2$N	6.2	5 99
CrN	6.05	6.14

Fig 4·4 : Av Mendeleev Number

61
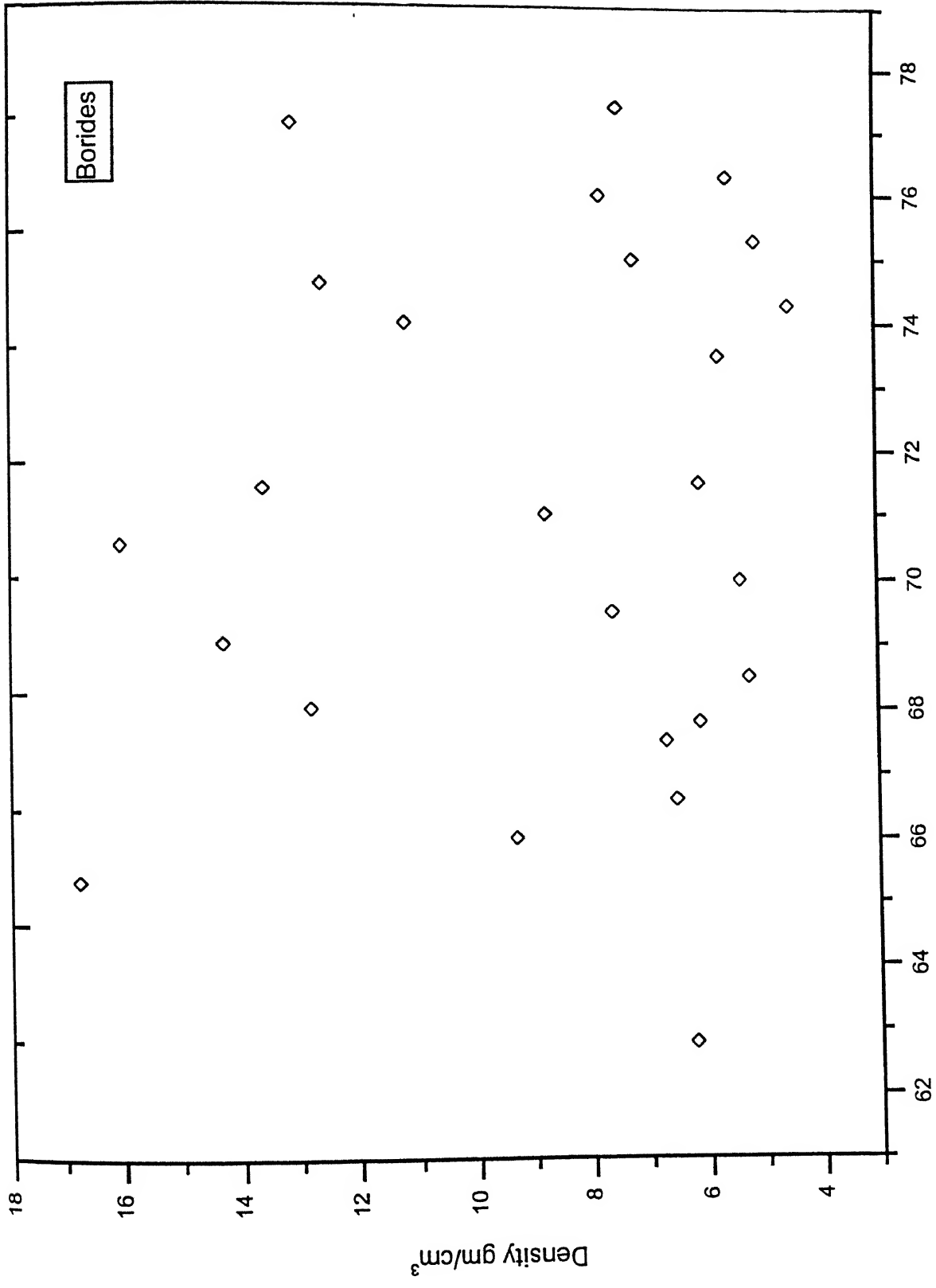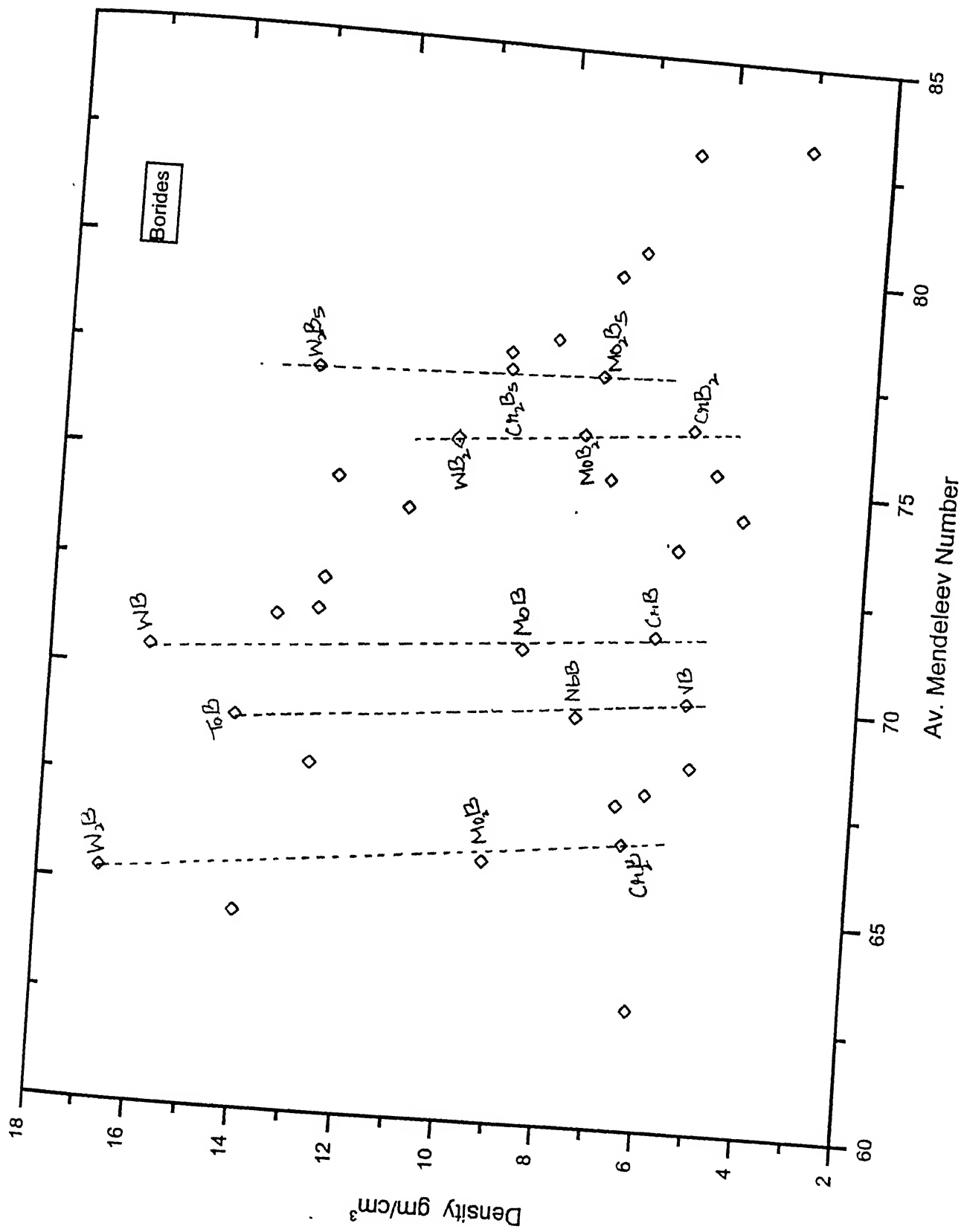
Fig. 4.5: Distribution of density of borides as a function of average mendeleev number
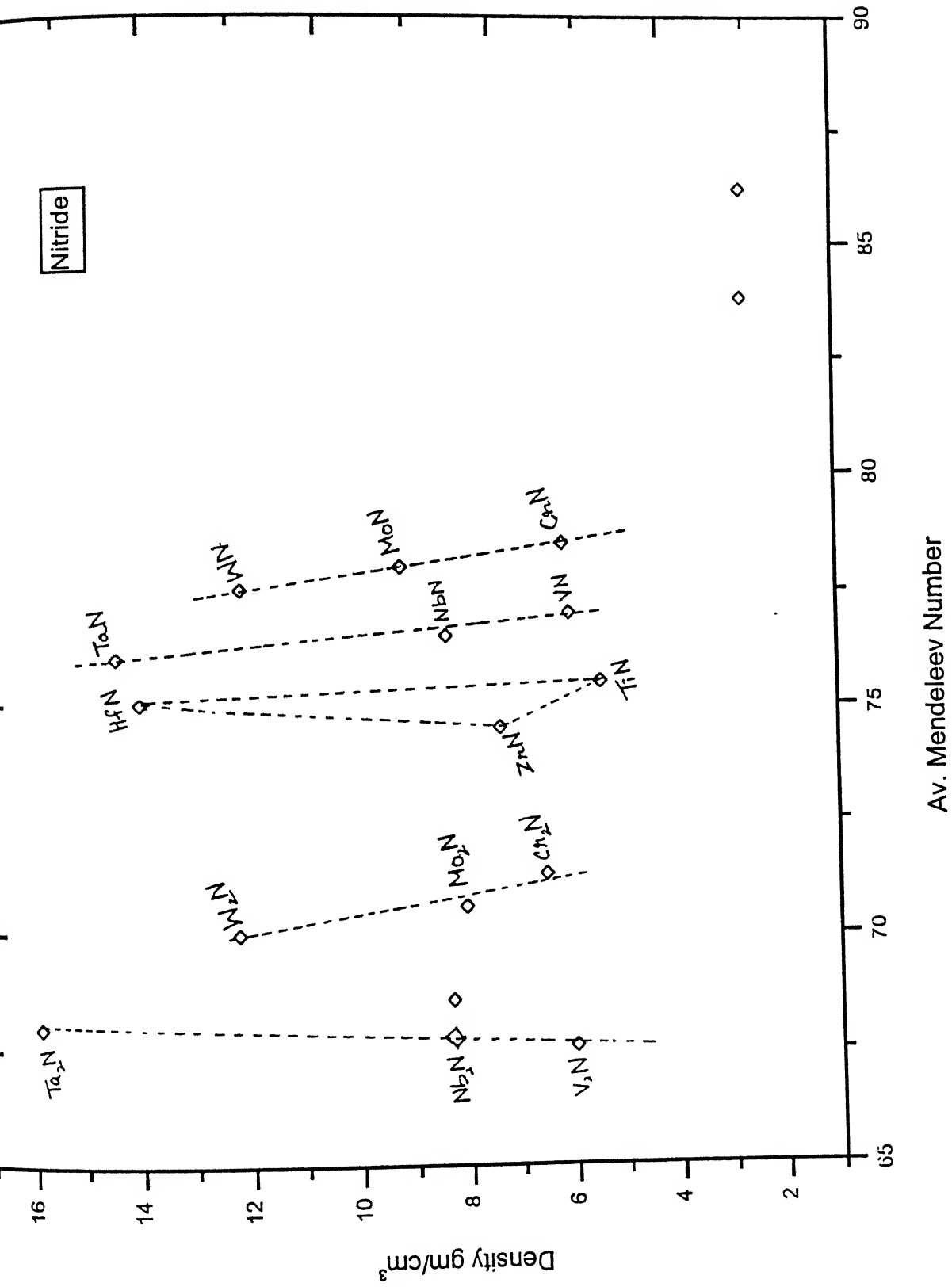
Fig.4.6: Distribution of density of nitrides as a function of average mendeleev number
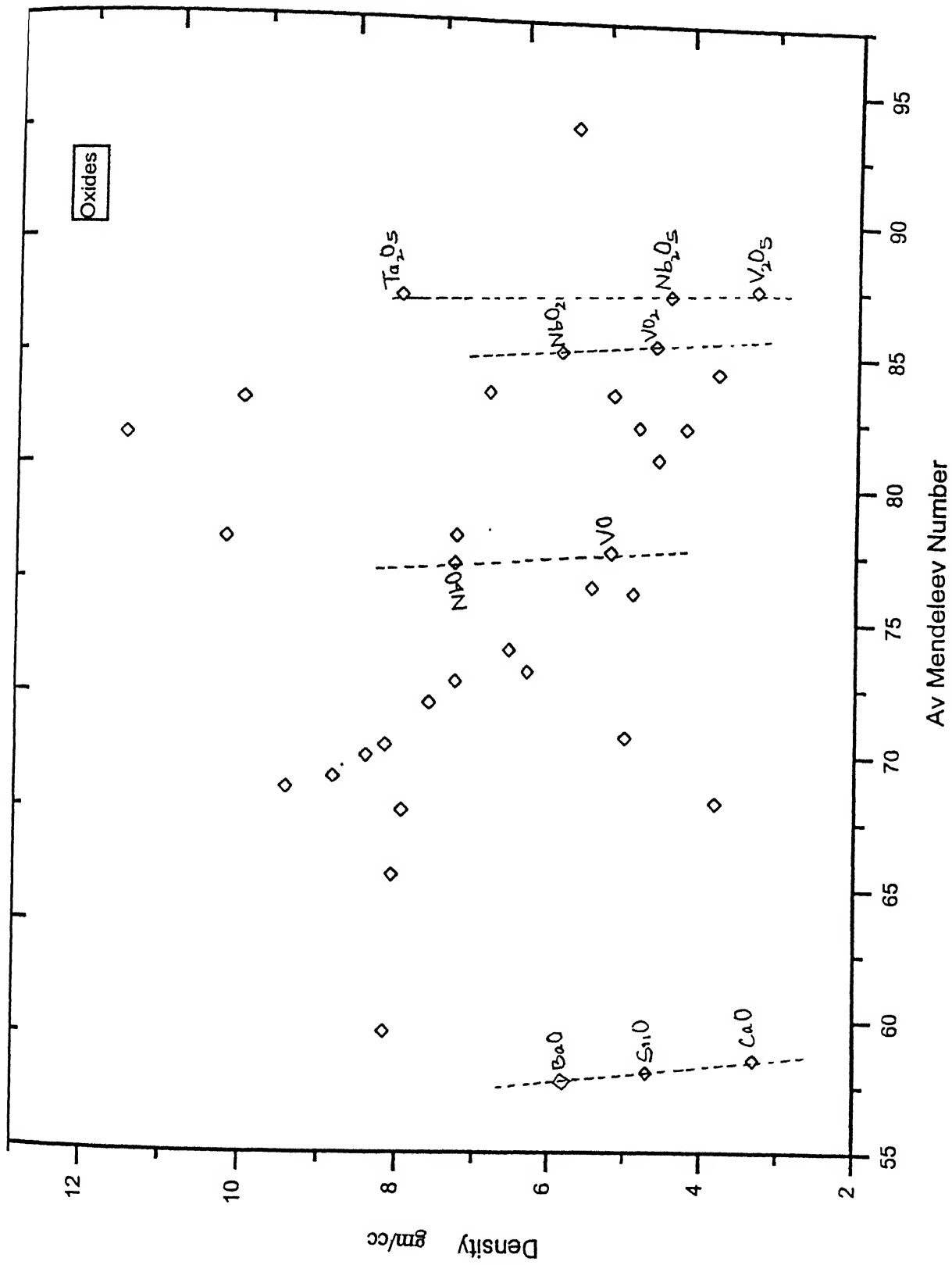
Fig.4.7: Distribution of density of oxides as a function of average mendeleev number
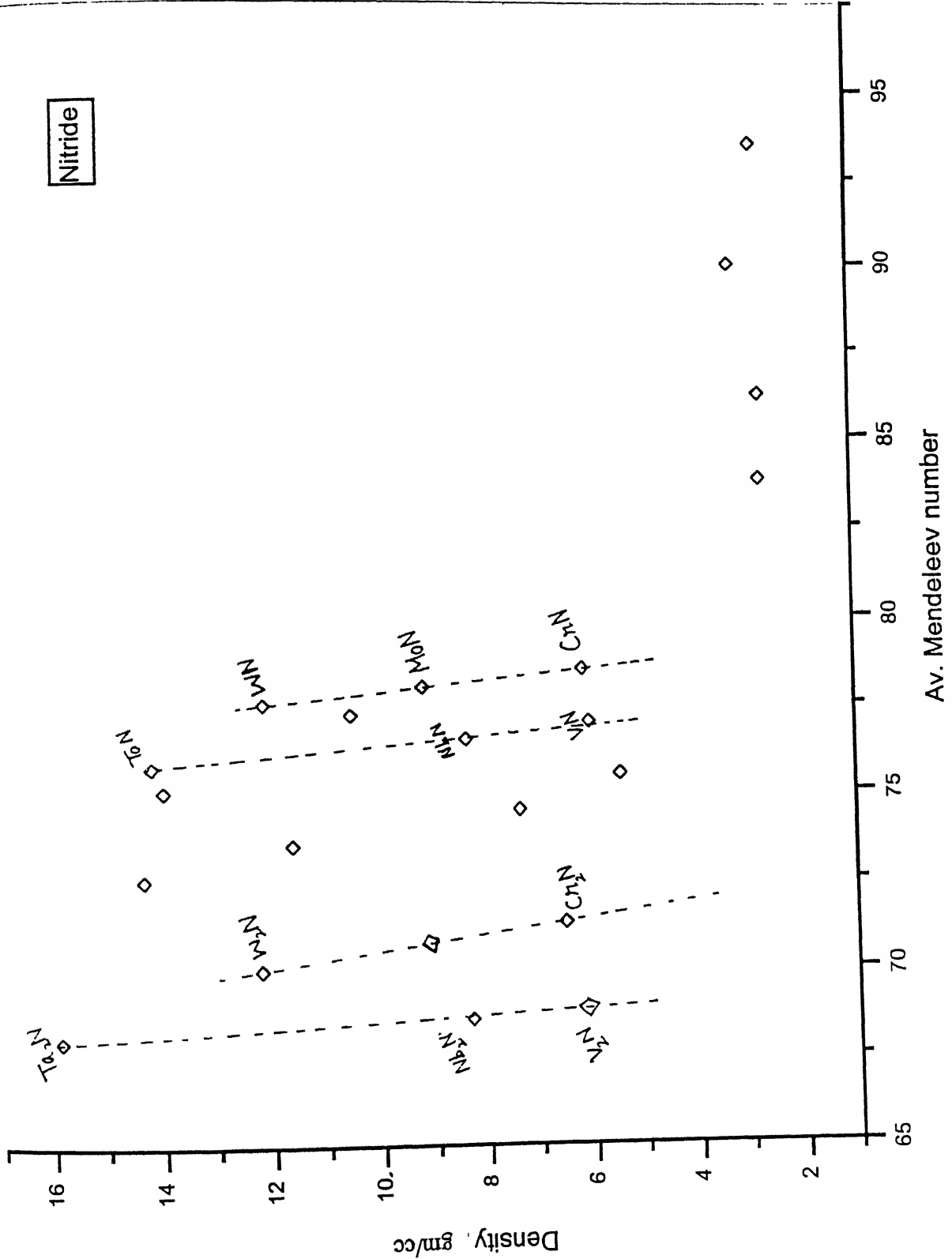
Fig.4.8: Distribution of density of nitrides as a function of average mendeleev number

4.3.1 Melting temperature verses Mendeleev number of some compounds

Fig 4 9 shows the distribution of melting temperature of oxides as a function of their average Mendeleev number M_A and melting temperature T_m of oxides has been taken from [38]. In Fig 4.10 we see some systematic (linear) patterns appearing in terms of position of groups of compounds: (W, Mo ,Cr)N, (W, Mo, *)₂N (*, V, Nb)₂ N, and (Be, *, Mg)₃N₂. Each straight line represents nitrides of particular type These missing compounds, which are denoted by '*' are Cr₂N, Ta₂N respectively We can also observe that all of these lines have similar slope The melting point temperature of unknown compound can be found by making use of geometrical similarity of these patterns. This requires first the calculation of the average Mendeleev numbers of unknown compounds. Using this approach the melting point temperature values for the missing compounds are shown in Table 4 2

Table 4.2: Calculated melting point temperature values of some compound

Name of the compound	Melting Temperature 'K	Literature Value K
IrO	1870	*
V₂N	2474	*
Cr₂N	1910	1725
Zn₃N₂	1875	*
Ta₂N	3180	3223

Other correlations can be obtained from fig.4.11. The Borides of Ta, Nb, V fall on straight lines with equal slopes. Each straight line represents a Boride of Particular type. These compounds are (Ta, Nb, V)B and (Ta, Nb, V)B₂. using the slope

We can find unknown density values for similar types of Borides.

Fig.4.9: Distribution of melting point temperature of borides as a function of average mendeleev number
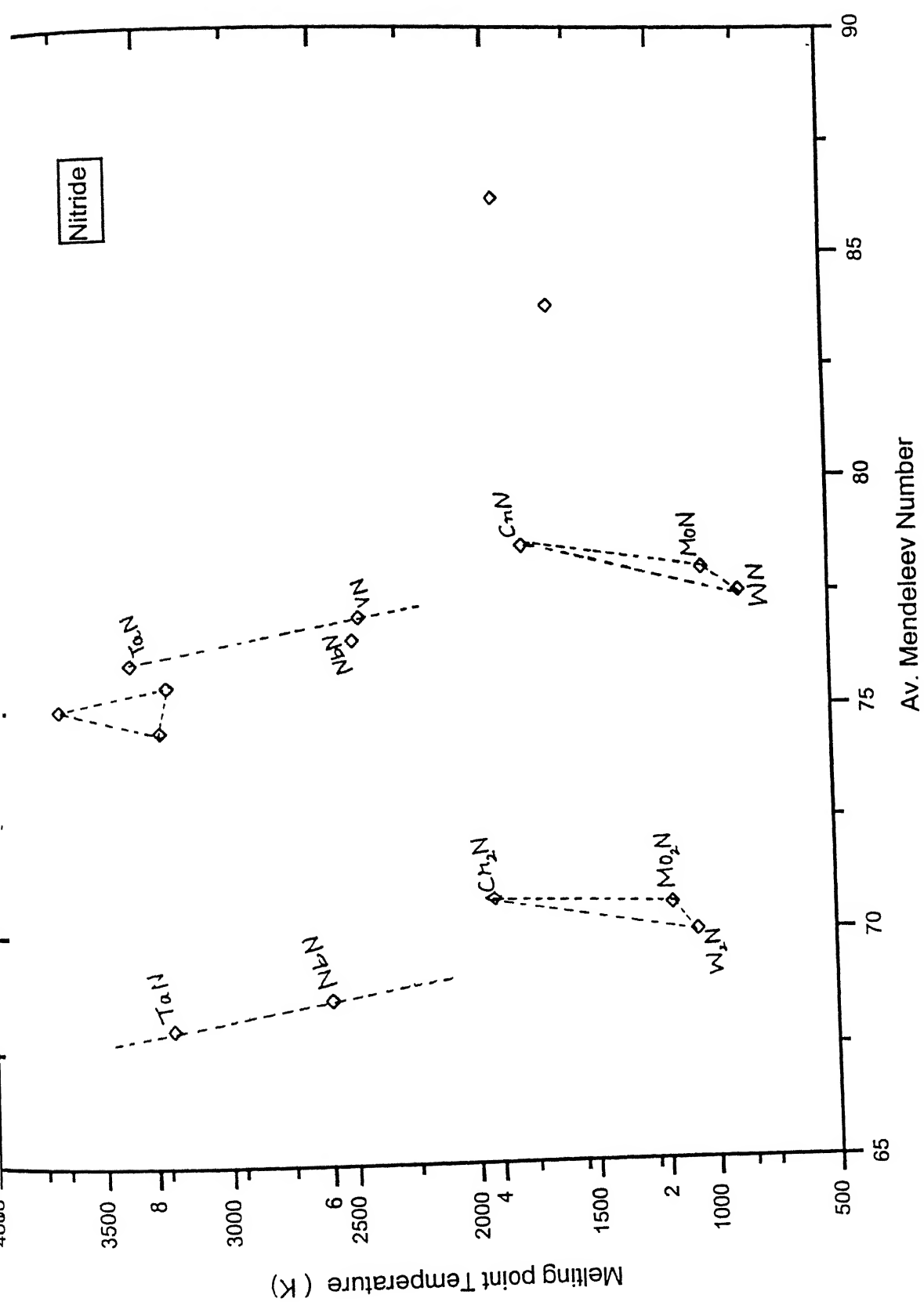
Fig.4.10: Distribution of melting point temperature of nitrides as a function of average mendeleev number
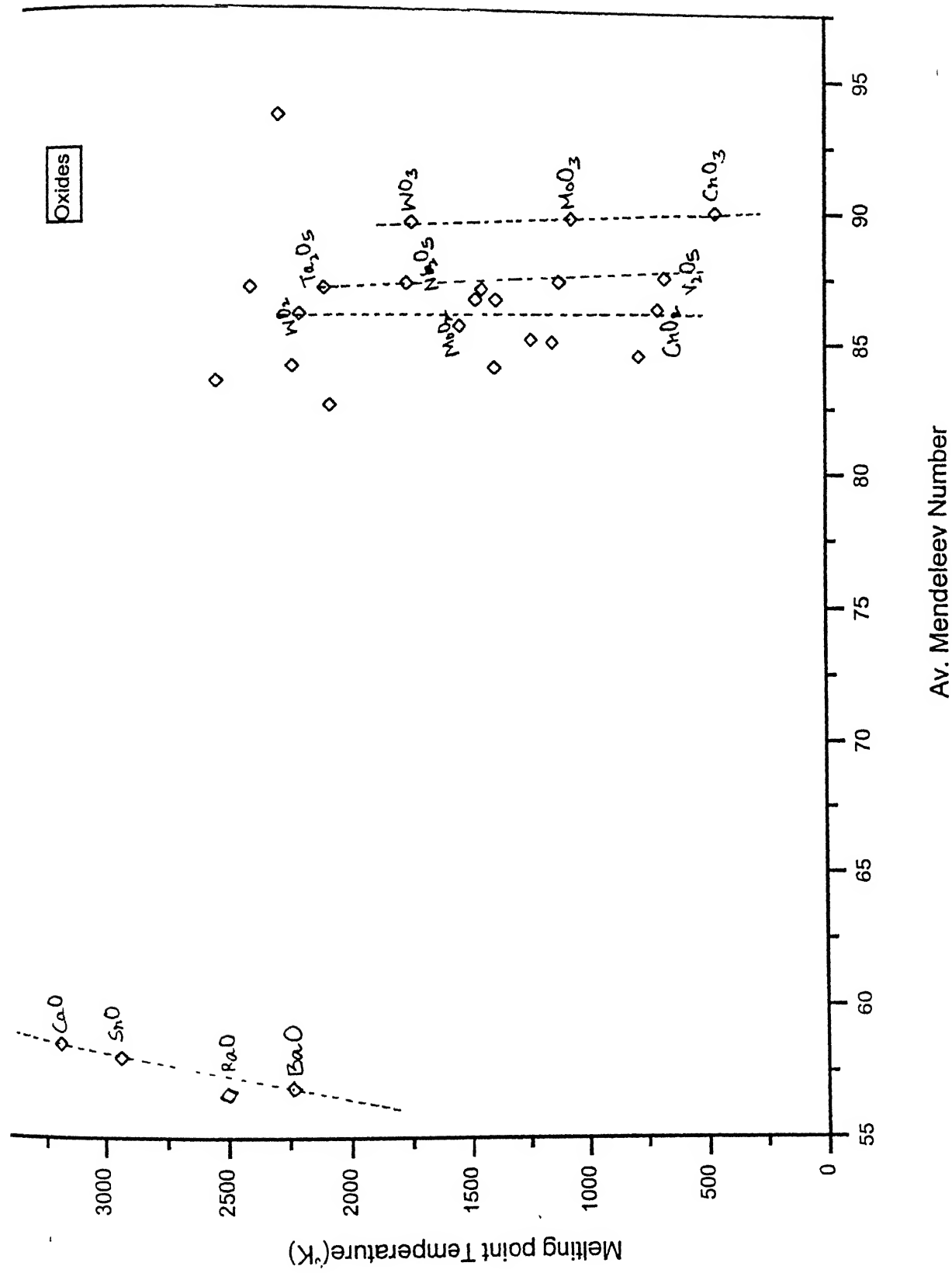
Fig.4.11: Distribution of melting point temperature of oxides as a function of average mendeleev number

Chapter 5

Property Estimation Using Neural Network

In the earlier chapter, we have considered estimation of property data using property ranges and correlations based on physical and empirical interrelation in things, structure maps etc. In this chapter we explore the possibility of using artificial neural network for this purpose.

5.1 Brief Introduction to Neural Network

People and animals are much better and faster at recognizing images than most advanced computers. Although computers outperform both biological and artificial neural systems for tasks based on precise and fast airthematic operations artificial neural systems represent the promising new generation of information processing networks.

Artificial neural systems function as parallel distributed computing networks. Their most basic characteristic is their architecture. Only some of the networks

provide instantaneous responses. Other networks need time to respond and are Characterized by their time domain behavior. Neural networks also differ from each other in their learning modes. Their are variety of learning rules that establish when and how the connecting weights change. Finally networks exhibit different speeds and efficiency of learning.

In contrast to conventional computers which are programmed to perform specific tasks most neural networks must be taught or trained. They learn new associations new patterns and new functional dependencies. Learning corresponds to parameter changes. Learning rules and algorithms used for experiential training of networks replace the programming required for conventional computation.

Neural network users do not specify an algorithm to be executed by each computing node. Instead they select what in their view is the best architecture, specify the characteristics of the neurons and initial weights and choose the training mode for the network. Appropriate inputs are then applied to the network so that it can acquire knowledge from the environment.[39]

Neural networks are developed to model the way in which the human brain performs a particular task . A neural network is a massively parallel distributed processor that has a natural propensity for storing experimental knowledge and making it available for use. The neural network provides a new type of computer architecture in which knowledge is acquired and stored over time through the use of adaptive learning algorithms. It resembles the brain in two respects.

(1) Knowledge is acquired by the network through a learning process.
(2) Interneuron connection strengths known as synaptic weights are used to store the knowledge

A neural is defined by three features topology, functioning and learning. Topology refers to the number of layers, number of nodes in each layer and the way nodes are connected. Functionality refers to the transfer function and discriminatory function of each node and the cost function of the network outputs .Learning refers to the learning algorithm and the values of learning parameters(learning rates and momentum). Learning rules specify an initial set of things and indicate how weights should be adapted during use to improve performance of neural network system.[45]

Neural networks can be classified differently according to different criteria the type of learning (supervised, unsupervised, self supervised) the mode of operation (on line, off line) the network interconnection architecture (feed forward , feedback recurrent) the number of layers the learning algorithm (Hebbian, back propagation resonant, Widrow Hoff).

The most forward neural network topology is feed forward networks, Multilayer Perceptron back propagation.

5.2   Simulation Procedure

The object of the simulation using neural network was to first have the system learn the appropriate mappings between input and output variables by observing the training samples The trained system was then used to determine the network Thus having an overview of neural network we will now use neural network approach for property relations in

- Carbides
- Nitrides
- Oxides
- Refractory compounds

We can apply neural network approach in our case because

- Correlations are empirical in nature
- Quality of correlations improves as we go on adding new additional inputs
- Correlations evolve in dynamic sense

The simulation were carried out using a Neural Network program [Easy NN][47] using the default algorithm and procedures for selecting weights

5.3 Results and Disscusion

Various simulations were carried out. The results can be summarized as follows. As discussed in [49], incorporating information about known correlations between the various variables in conjunction with neural network result in improved estimates. Accordingly results based on the "informed neural network" approach are also estimated and compared.

5.3.1 Carbides

A. Estimation of Hardness and G

Input Variables: Density (gm/cc), Melting Temperature (K), Elastic modulus(10^5Nmm^{-2}). The simulation for "informed neural network" includes an additional input variable c_2E based on the correlation $GE=c_2$ where $c_2=0.4209$

Output Variables: Hardness, G

Training Pair and query data: as per Table 5.1

WC	By property ranges	By Neural Network	By Informed Neural Network	Literature value
H Error		Software cannot extrapolate	Software cannot extrapolate	3100
G(10^5Nmm$^{1/2}$) Error	241.93 .02%	Software cannot extrapolate	Software cannot extrapolate	242

B. Estimation of Hardness and thermal expansion coefficient

   Input Variables: Density (gm/cc), Melting Temperature (K), Elastic modulus(10^5Nmm^{-2}).The simulation for "informed neural network" includes an additional input variable αT_m based on the correlation $\alpha T_m = c_1$ where $c_1 = 17752.7$

   Output Variables: Hardness, α

   Training Pair: as per Table 5.2

WC	By property ranges	By Neural Network	By Informed Neural Network	Literature value
H	-	1517 51%	1759 43%	3100
α Error	5.49 9%	5.8 16%	5.68 13%	5

The neural network is shown in figure 5.2

C. The above simulations (A&B) were run again to estimate property data for ZrC with WC included as training data the results obtained (from the two runs) were as follows. The results for hardness estimates are not given since no comparisons can be made in the absence of appropriate correlations.

ZrC	By property ranges	By Neural Network	By Informed Neural Network	Literature value
$\alpha(10^{-6}K^{-1})$ Error	5.49 8%	5.68 5%	5.8 3%	6
$G(10^5Nmm^{1/2})$ Error	1.39 1.4%	1.485 5.3%	1.4612 5.1%	1.41

The training data and query data are shown in Table 5.1(continued). The neural network model is shown in figures 5.1 and 5.2

5.3.2 Nitrides

   Input Variables: Density (gm/cc), Melting Temperature (K), Elastic modulus(10^5Nmm^{-2}) The simulation for "informed neural network" includes an additional input variable c_1/T_m based on the correlation $\alpha\, T_m = c_1$ where $c_1 = 11261.74$.

Output Variables: Hardness, Linear thermal expansion(10^{-6} K^{-1})

Training Pair: Aluminum nitride, Boron nitride, Chromium nitride, Titanium nitride etc.

Query data:

VN	By property ranges	By Neural Network	By Informed Neural Network	Experimental value
α (10^{-6}K^{-1})	7.0	10 09	9.35	8.9
Error		13%	5%	
Hardness	-	2492.7	1414.5	1520
Error		63%	6.9%	

The training data and query data are shown in Table 5.2. The calculation of different properties is done in Chapter 3. Neural network model for above problem is shown in Fig. 5.2

5.3.3 Oxides

Input Variables: Density(gm/cc), Melting temperature(K), Elastic modulus(10^5 Nmm^{-2})

Output Variables: Hardness, Linear thermal expansion(10^{-6} K^{-1})

Training pair: BeO, MgO, SiO$_2$, NiO etc.

Query data:

ZrO$_2$	By property ranges	By Neural Network	By Informed Neural Network	Literature value
Hardness	-	1072		1200
Error		10%		
G(10^5Nmm$^{1/2}$)	58	57.87	59.02	60
Error	3%	3%	1.6%	
α(10^{-6}K^{-1})	7.73	8.08	7.7	7.5
Error	3%	7%	2.6%	

The training data and query data are given in Table 5.3. The calculation of different properties is done in Chapter 3 Neural network model for above problem is shown in Fig 5 3

5.3.4 Refractory Compounds

Input Variables: Mendeleev Number(A) , Valency(A), Mendeleev Number(B), Valency(B).
Where A is a constituent element. And B represents Boride, Carbide, Nitride or Oxide.

Output Variable: Density(gm/cc) , Melting point temperature (K)

Training pair: carbides, borides ,nitrides and oxides (see Table5.5)

Query data:

Refractory Compound*	Density(gm/cc)*	Melting point temperature(K)*
VN	6.02(6.68)	2450(2311.37)
NbN	8.36(8.61)	2477(2606)
TaN	14.36(13.83)	3366(3444)

(* Neural Network output values are given in bracket and compared with literature value)

The training data and query data are given in Table 5.4 while the comparison of query values with the literature values is given as above . The neural network model for above problem is shown in Fig.5.4. The results presented in the preceding sections indicate that neural networks is an effective tool for estimating unknown property data. The results are generally comparable to estimates made using correlations approach as shown earlier [49], the "informed neural network" approach always yields more accurately results compared the neural network approach.
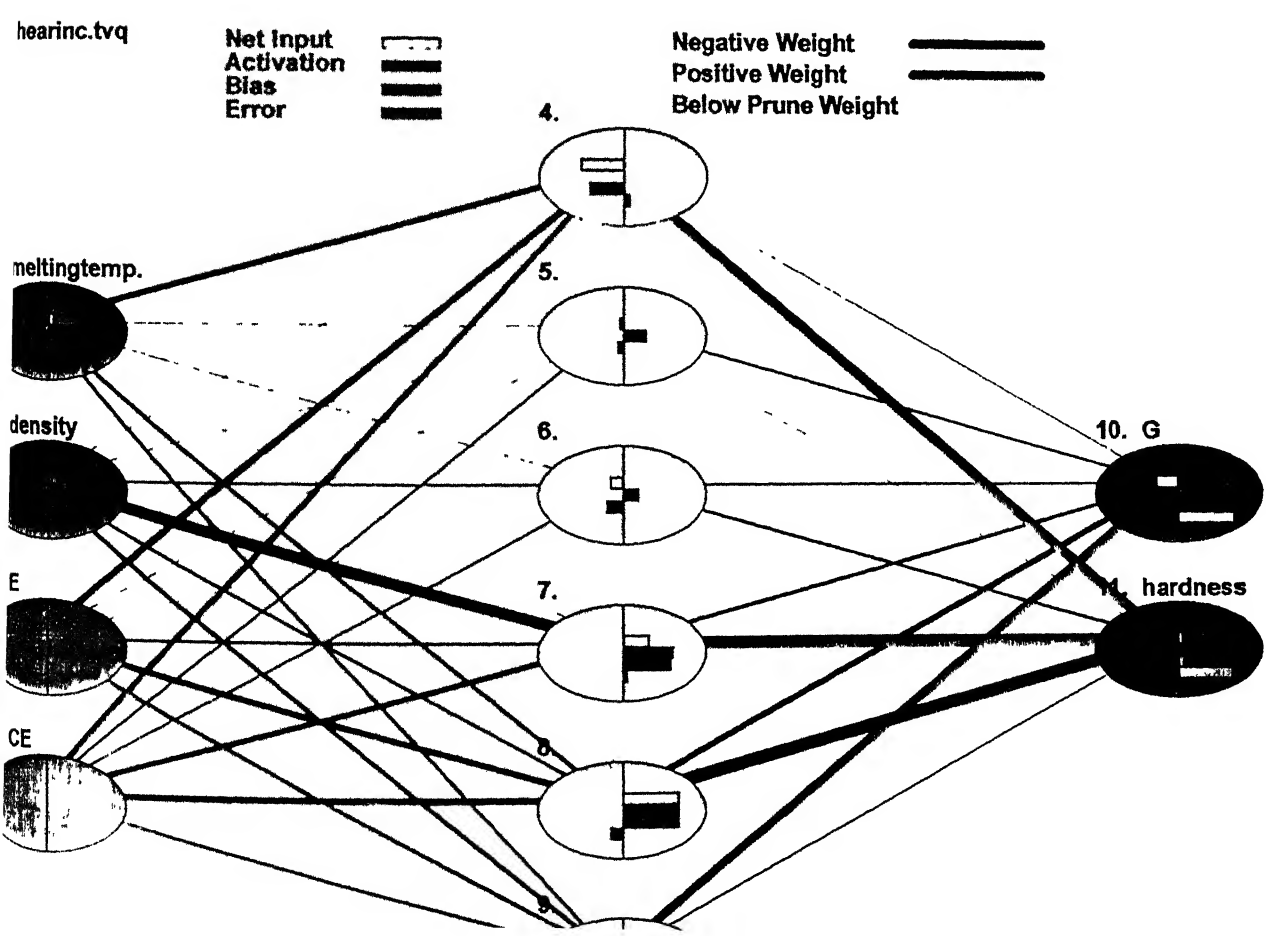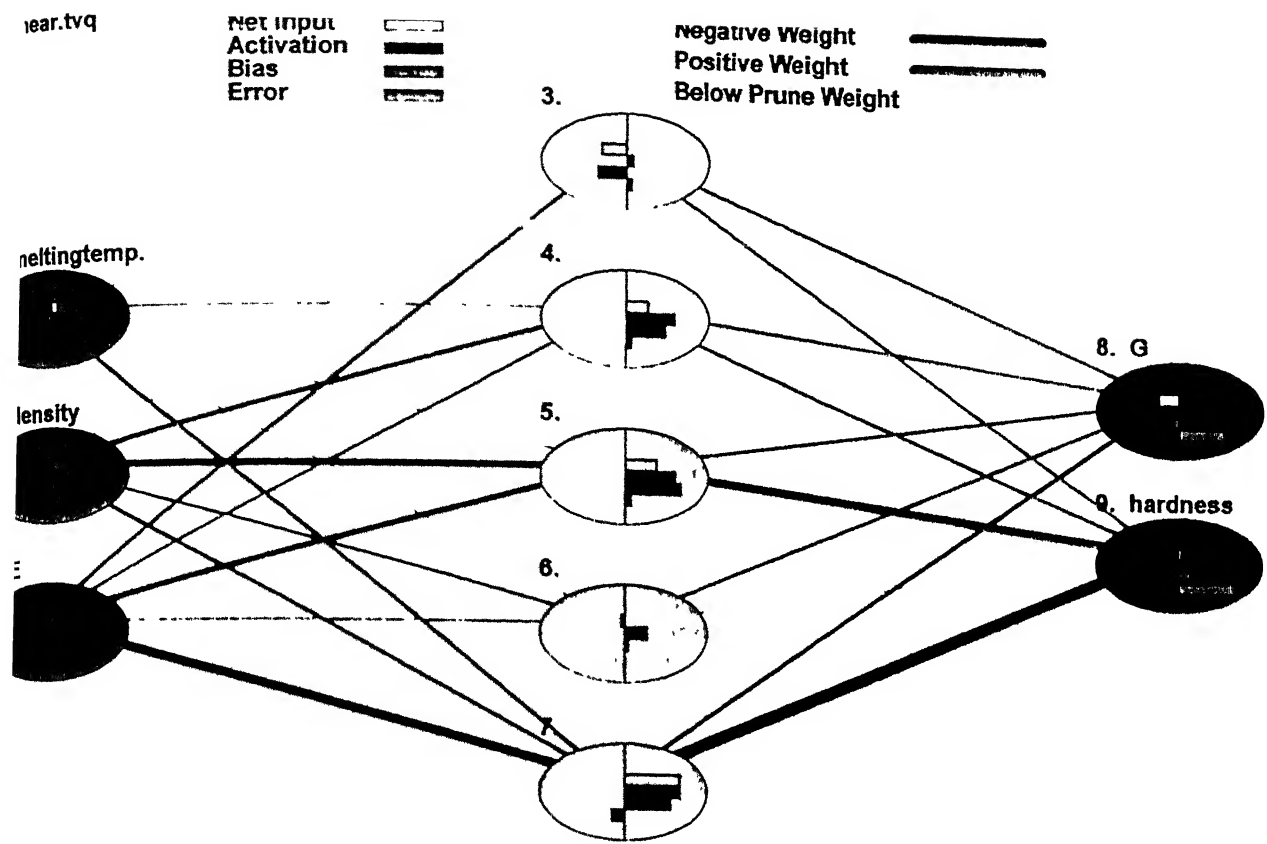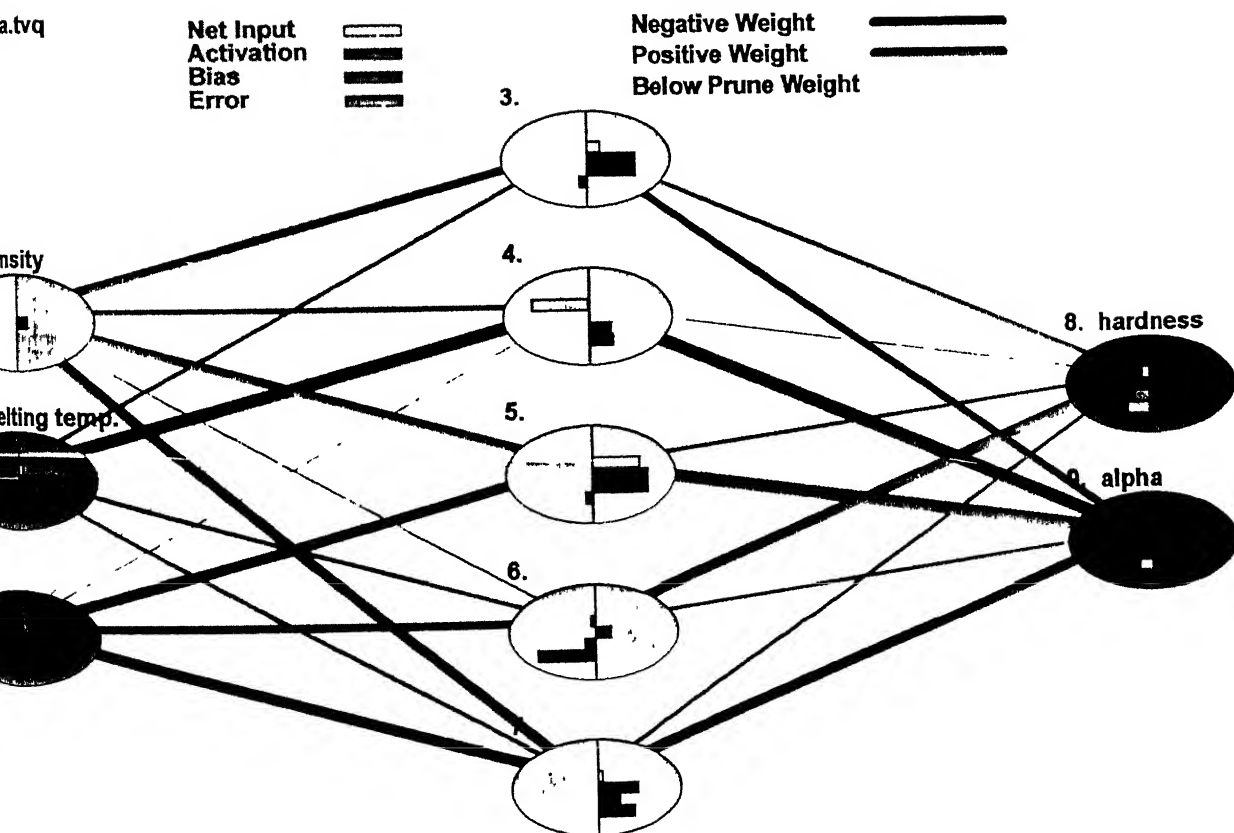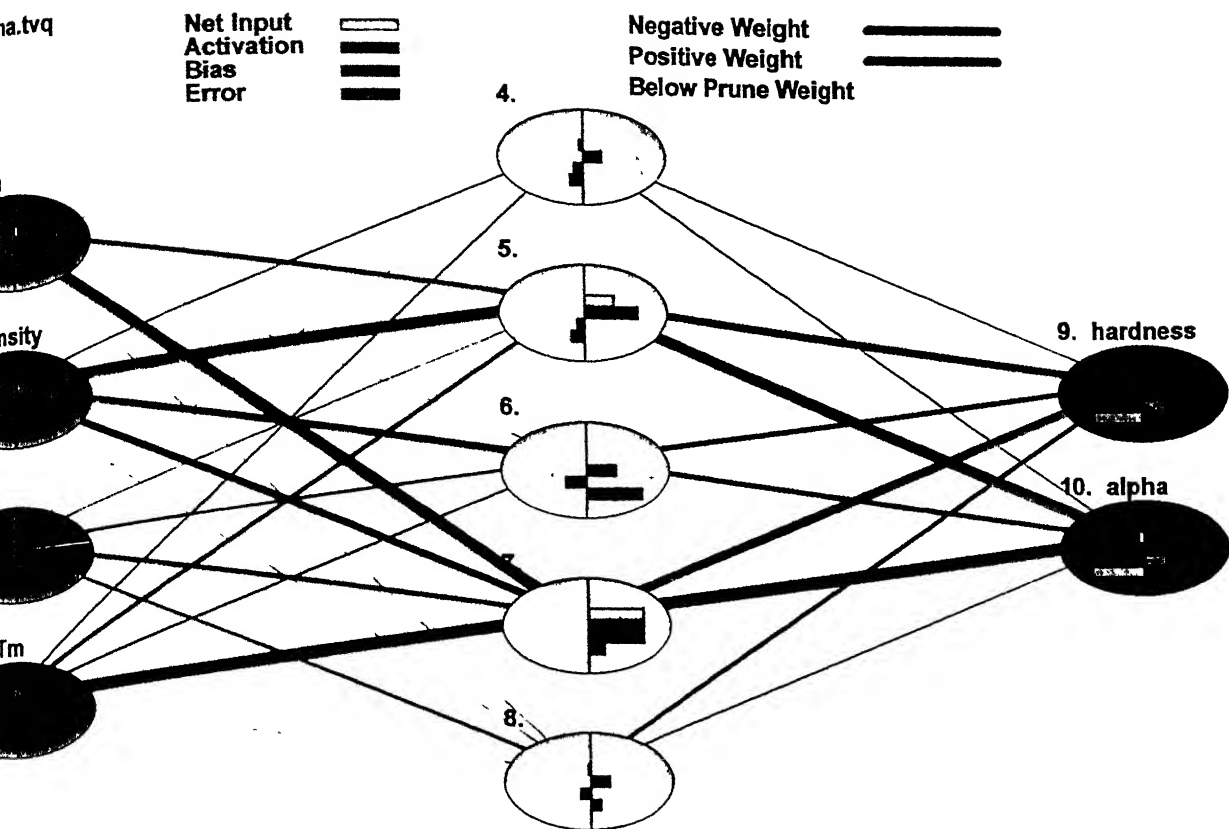
1.tvq

Net Input
Activation
Bias
Error
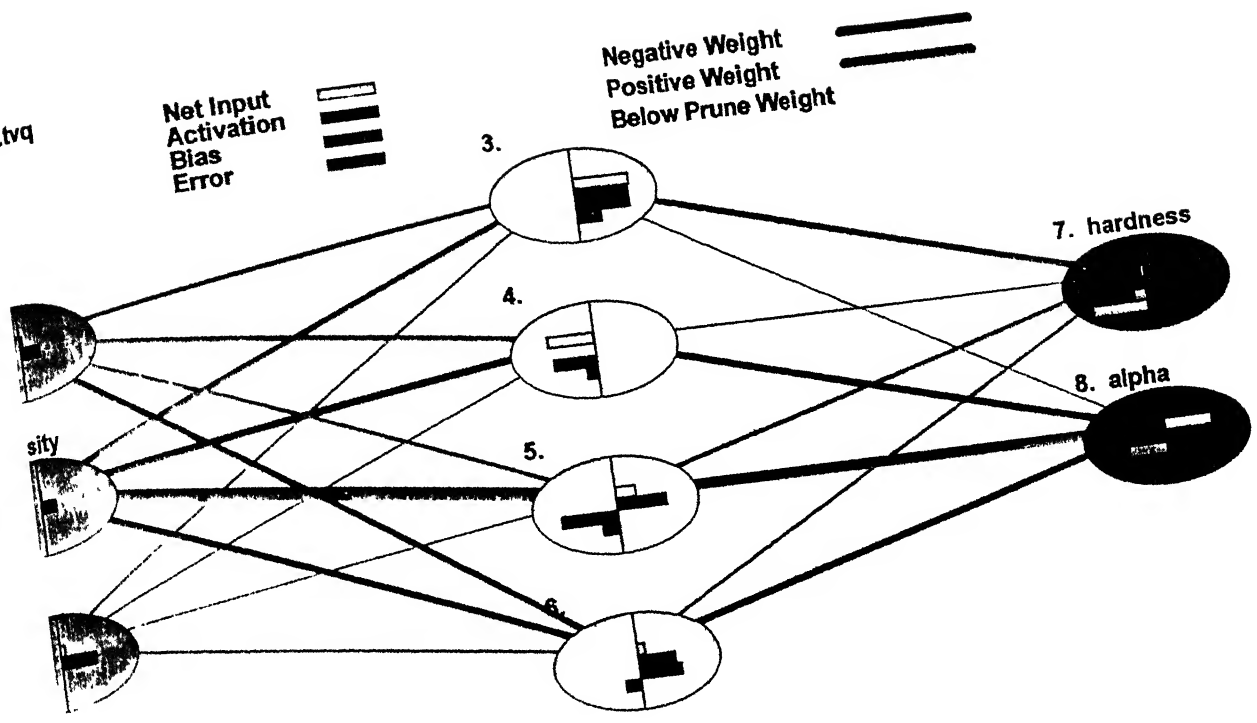
Negative Weight
Positive Weight
Below Prune Weight

3.

4.

5.

6.

sity

7. hardness

8. alpha

2.tvq

Net Input
Activation
Bias
Error

Negative Weight
Positive Weight
Below Prune Weight

4.

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nsity

Tm

10. hardness

11. alpha
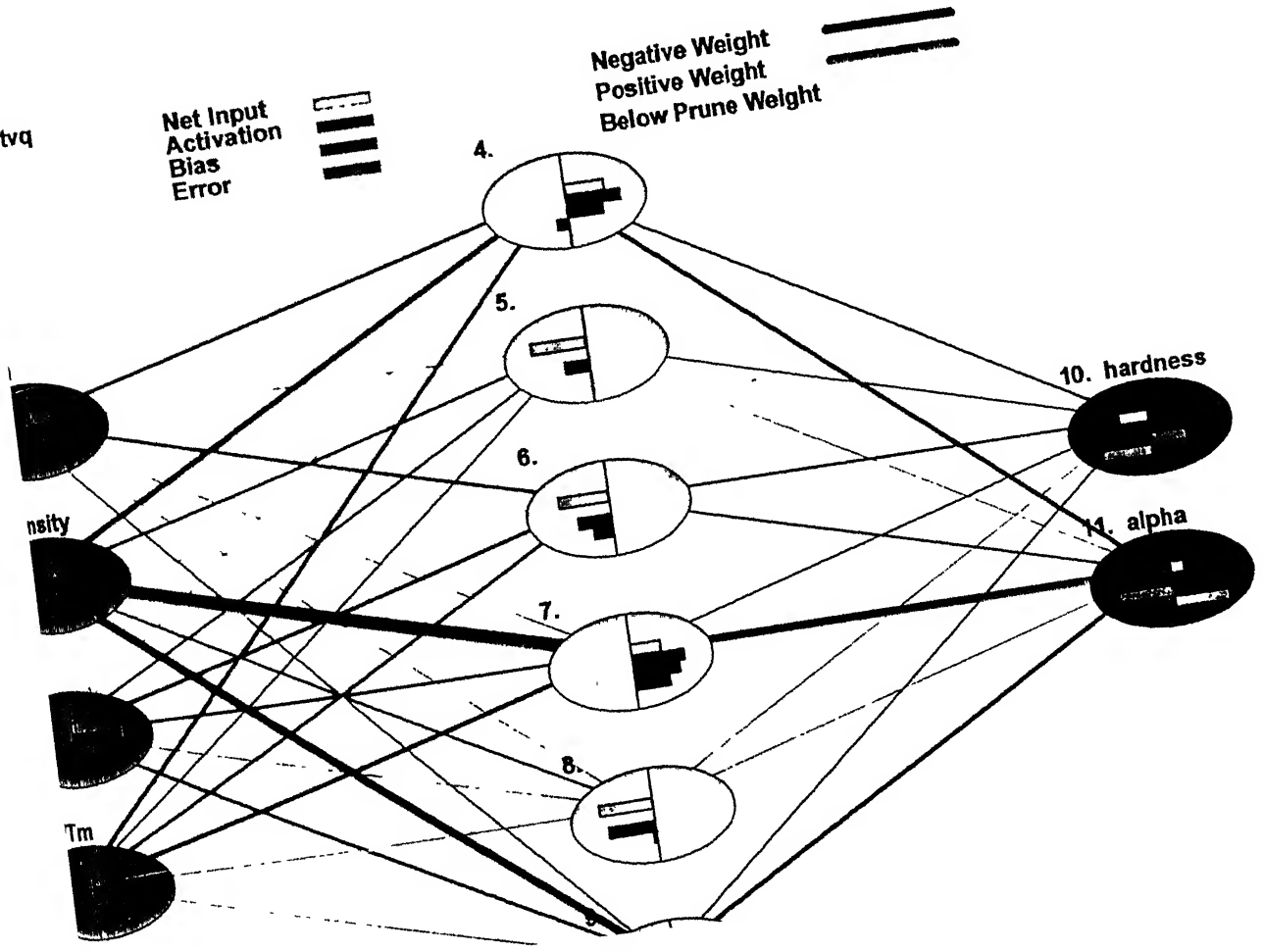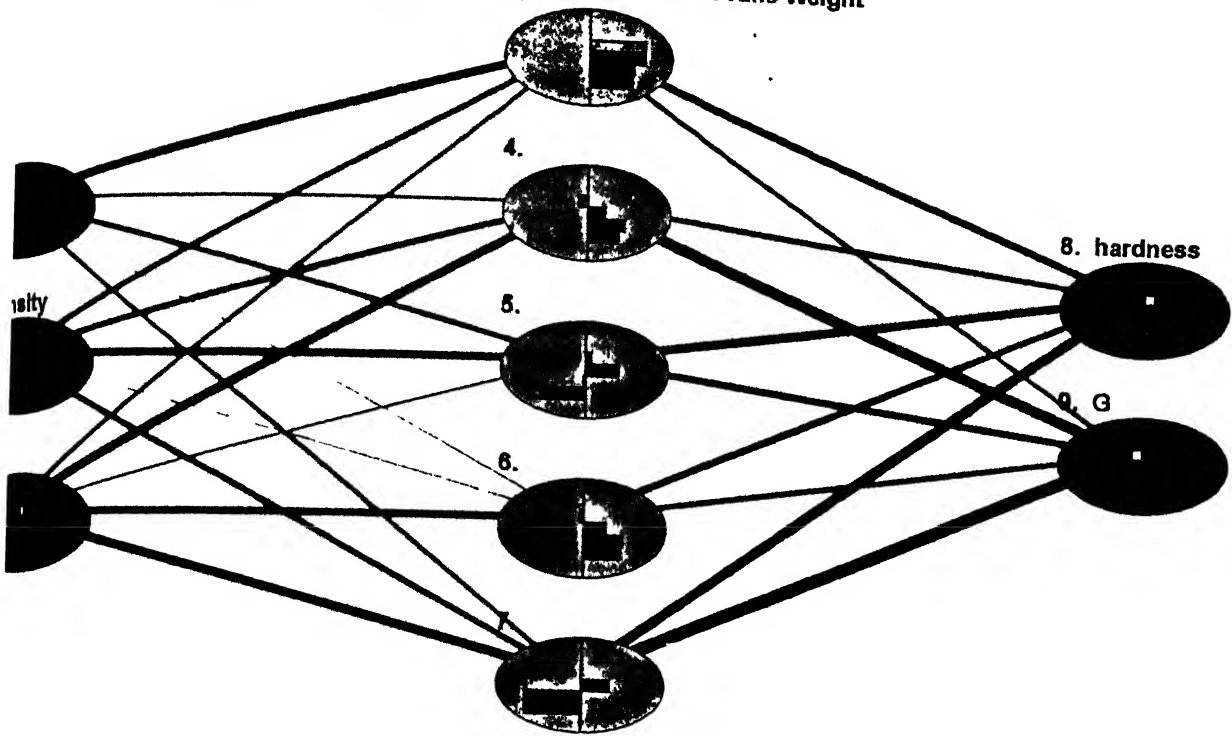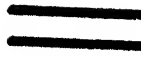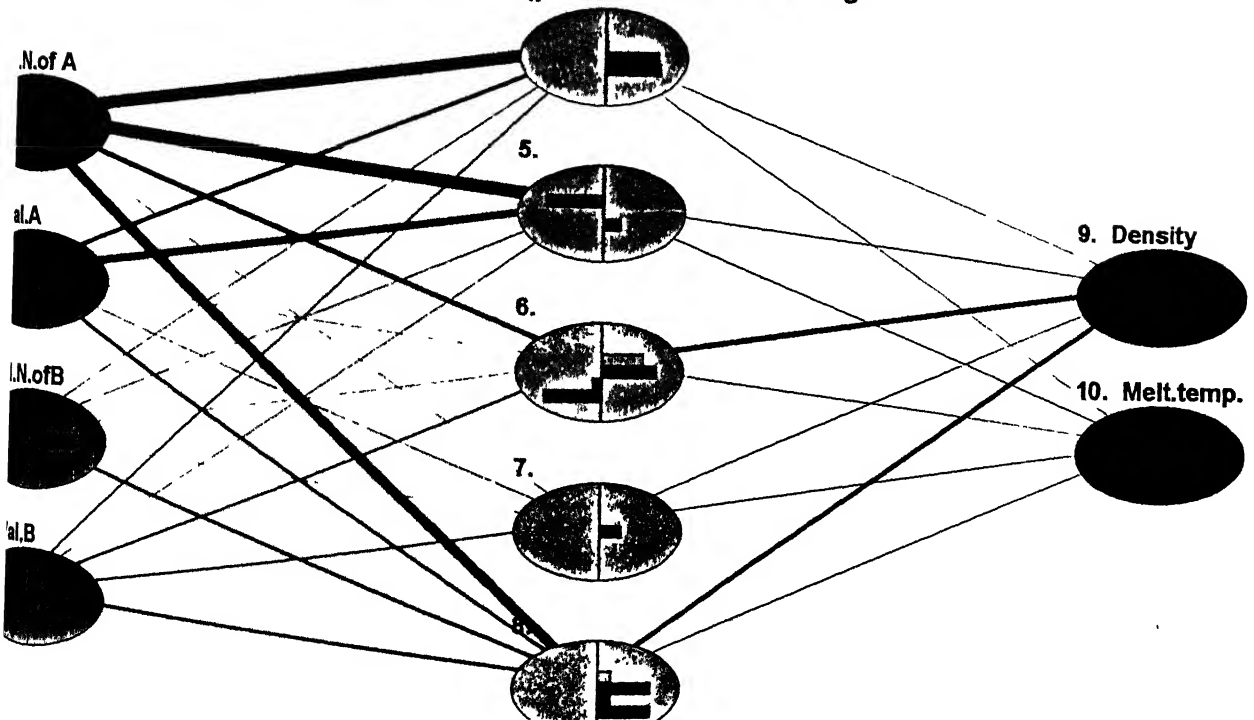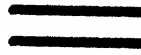
: meltingtemp.	2400.0000	O: G	1.8600
: density	2.4500	O: hardness	3100.0000
: E	4.4000		
: CE	1.8520		

: meltingtemp.	3770.0000	O: G	1.2900
: density	7.6000	O: hardness	2300.0000
: E	3.2000		
: CE	1.3470		

: meltingtemp.	2970.0000	O: G	1.7500
: density	3.0000	O: hardness	2500.0000
: E	3.9000		
: CE	1.6420		

: meltingtemp.	4050.0000	O: G	1.4500
: density	13.4000	O: hardness	1300.0000
: E	3.6000		
: CE	1.5771		

: meltingtemp.	3440.0000	O: G	1.6500
: density	4.9000	O: hardness	2500.0000
: E	4.2000		
: CE	1.7680		

I: meltingtemp.	3090.0000	O: G	2.4300
I: density	15.5000	O: hardness	3100.0000
I: E	6.0000		
I: CE	2.5260		

I: meltingtemp.	3300.0000	O: G	1.4612
I: density	6.6000	O: hardness	2345.5124
I: E	3.4600		
I: CE	1.2171		

	Value			Value
"	150.0000	O: hardness		
density	.5200	O: alpha		c 00
E	1.5000			
C/Tm	7.2640			
Tm	1900.0000	O: hardness		1500.0000
density	6.6800	O: alpha		10.0000
E	4.0000			
C/Tm	9.3660			
Tm	1780.0000	O: hardness		2200.0000
density	6.9000	O: alpha		10.0000
E	3.5000			
C/Tm	4.9980			
Tm	3830.0000	O: hardness		2200.0000
density	12.2000	O: alpha		6.3000
E	3.5500			
C/Tm	4.6460			
Tm	3490.0000	O: hardness		2400.0000
density	7.7800	O: alpha		6.6500
E	3.4000			
C/Tm	5.0990			
Tm	2200.0000	O: hardness		4500.000
density	.2000	O: alpha		5.6800
E	4.8000			
C/Tm	8.0890			
Tm	3780.0000	O: hardness		1790.000
density	14.5000	O: alpha		6.2900
E	6.2900			
C/Tm	4.7081			
Tm	3067.0000	O: hardness		3200.000
density	4.9300	O: alpha		7.4200
E	4.0000			
C/Tm	5.8026			
Tm	2830.0000	O: hardness		2950.000
density	5.5000	O: alpha		6.5000
E	2.8000			
C/Tm	6.2880			
Tm	2600.0000	O: hardness		1759.369
density	15.7000	O: alpha		5.6397
E	7.2000			
C/Tm	6.8440			
Tm	3535.0000	O: hardness		2654.23
density	6.5000	O: alpha		5.8562
E	3.8000			
C/Tm	5.0340			

I: density   3.0500   O: hardness
I: melting temp. 2200.0000 O: alpha   1200.0000
I: E   3.1500   6.0000

I: density   2.2500   O: hardness
I: melting temp. 3000.0000 O: alpha   4400.0000
I: E   0.9000   3.8000

I: density   6.1000   O: hardness
I: melting temp. 1050.0000 O: alpha   1800.0000
I: E   4.0000   2.3000

I: density   5.9000   O: hardness
I: melting temp. 1500.0000 O: alpha   2250.0000
I: E   3.1380   9.4000

I: density   13.8000   O: hardness
I: melting temp. 3310.0000 O: alpha   1700.0000
I: E   3.3300   6.9000

I: density   8.4000   O: hardness
I: melting temp. 2570.0000 O: alpha   1400.0000
I: E   4.8300   10.1000

I: density   3.4400   O: hardness
I: melting temp. 1900.0000 O: alpha   1410.0000
I: E   2.1000   2.4000

I: density   3.6000   O: hardness
I: melting temp. 3000.0000 O: alpha   3240.0000
I: E   5.7600   3.6000

I: density   5.2100   O: hardness
I: melting temp. 2950.0000 O: alpha   1997.123
I: E   2.5000   6.3257

: Tm	2200.0000	O: hardness	1200.0000
: density	2.2500	O: alpha	6.0000
: E	3.1500		

: Tm	3000.0000	O: hardness	4400.0000
: density	2.2500	O: alpha	3.8000
: E	0.9000		

: Tm	1050.0000	O: hardness	1800.0000
: density	6.1000	O: alpha	2.3000
: E	4.0000		

: Tm	1500.0000	O: hardness	2250.0000
: density	5.9000	O: alpha	9.4000
: E	3.1380		

: Tm	3310.0000	O: hardness	1700.0000
: density	13.8000	O: alpha	6.9000
: E	3.3300		

: Tm	2570.0000	O: hardness	1400.0000
: density	8.4000	O: alpha	10.1000
: E	4.8300		

4

: Tm	1900.0000	O: hardness	1410.0000
: density	3.4400	O: alpha	2.4000
: E	2.1000		

: Tm	3000.0000	O: hardness	3240.0000
: density	3.6000	O: alpha	3.6000
: E	5.7560		

: Tm	2950.0000	O: hardness	2450.0000
: density	5.2100	O: alpha	9.3500
: E	2.5000		

: Tm	2050.0000	O: hardness	2492.7096
: density	6.1300	O: alpha	10.0530
: E	4.6000		

: Tm	3000.0000	O: hardness	1345.117?
: density	6.9300	O: alpha	10.0974
: E	5.1000		

: Tm	?	O: hardness	?
: density	?	O: alpha	?
: E	0.0000		

I: Tm	2200.0000	O: hardness	1200.0000
I: density	2.2500	O: alpha	6.0000
I: E	3.1500		
I: C/Tm	5.1190		

I: Tm	3000.0000	O: hardness	4400.0000
I: density	2.2500	O: alpha	3.8000
I: E	0.9000		
I: C/Tm	3.7530		

I: Tm	1050.0000	O: hardness	1800.0000
I: density	6.1000	O: alpha	2.3000
I: E	4.0000		
I: C/Tm	10.7200		

I: Tm	1500.0000	O: hardness	2250.0000
I: density	5.9000	O: alpha	9.4000
I: E	3.1380		
I: C/Tm	7.5070		

I: Tm	3310.0000	O: hardness	1700.0000
I: density	13.8000	O: alpha	6.9000
I: E	3.3300		
I: C/Tm	3.4020		

I: Tm	2570.0000	O: hardness	1400.0000
I: density	8.4000	O: alpha	10.1000
I: E	4.8300		
I: C/Tm	4.3820		

I: Tm	1900.0000	O: hardness	1410.0000
I: density	3.4400	O: alpha	2.4000
I: E	2.1000		
I: C/Tm	5.9270		

I: Tm	3000.0000	O: hardness	3240.0000
I: density	3.6000	O: alpha	3.6000
I: E	5.7560		
I: C/Tm	3.7530		

I: Tm	2950.0000	O: hardness	2450.0000
I: density	5.2100	O: alpha	9.3500
I: E	2.5000		
I: C/Tm	3.8175		

I: Tm	2050.0000	O: hardness	1414.5074
I: density	6.1300	O: alpha	9.0569
I: E	4.6000		
I: C/Tm	5.4930		

I: Tm	3000.0000	O: hardness	1345.1179
I: density	6.9300	O: alpha	10.0974
I: E	5.1000		
I: C/Tm	3.7539		

| | | O: hardness | ? |

l2O3
I: Tm	2320.0000	O: hardness		1500.0000
I: density	3.7500	O: G		1.0000
I: E	3.3000			

aO
I: Tm	2820.0000	O: hardness		1100.0000
I: density	2.8000	O: G		1.1700
I: E	3.4000			

gO
I: Tm	3080.0000	O: hardness		500.0000
I: density	3.5400	O: G		0.9200
I: E	2.7000			

rO2
I: Tm	2950.0000	O: hardness		1072.0000
I: density	5.7000	O: G		0.5700
I: E	1.8000			

iO2
I: Tm	1703.0000	O: hardness		1091.2571
I: density	2.3300	O: G		0.9277
I: E	6.9000			

hO
I: Tm	2263.0000	O: hardness		0.0000
I: density	6.6700	O: G		3.4200
I: E	9.5800			

hO2
I: Tm	3478.0000	O: hardness		950.0000
I: density	10.0000	O: G		0.0000
I: E	1.3800			

fO2
I: Tm	2900.0000	O: hardness		?
I: density	9.7000	O: G		?
I: E	0.0000			

Table 5.4: Training and query data for oxides

M.N.of A	51.0000	O: Density	5.2600
Val.A	4.0000	O: Melt.temp.	2323.0000
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	49.0000	O: Density	6.7000
Val.A	4.0000	O: Melt.temp.	0.0000
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	50.0000	O: Density	12.8000
Val.A	4.0000	O: Melt.temp.	3172.0000
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	54.0000	O: Density	5.4000
Val.A	3.0000	O: Melt.temp.	2522.0000
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	53.0000	O: Density	7.6000
Val.A	3.0000	O: Melt.temp.	2533.0000
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	52.0000	O: Density	14.2900
Val.A	3.0000	O: Melt.temp.	2760.0000
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	57.0000	O: Density	2.8000
Val.A	2.0000	O: Melt.temp.	3136.4275
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	56.0000	O: Density	7.8555
Val.A	2.0000	O: Melt.temp.	3309.5345
M.N.ofB	86.0000		
Val.B	5.0000		
M N.of A	55.0000	O: Density	14.3600
Val.A	2.0000	O: Melt.temp.	3201.6637
M.N.ofB	86.0000		
Val.B	5.0000		
M.N.of A	51.0000	O: Density	4.9000
Val.A	4.0000	O: Melt.temp.	3440.0000
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	49.0000	O: Density	6.6000
Val.A	4.0000	O: Melt.temp.	3300.0000
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	50.0000	O: Density	12.6700
Val.A	4.0000	O: Melt.temp.	4203.0000

M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	54.0000	O: Density	13.6000
Val.A	3.0000	O: Melt.temp.	2769.0000
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	53.0000	O: Density	7.6000
Val.A	3.0000	O: Melt.temp.	3770.0000
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	52.0000	O: Density	13.5482
val.A	3.0000	O: Melt.temp.	3846.7107
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	56.0000	O: Density	14.1609
Val A	2.0000	O: Melt.temp.	3978.8412
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	55.0000	O: Density	14.2715
Val.A	2.0000	O: Melt.temp.	4027.4925
M.N.ofB	95.0000		
Val.B	4.0000		
M.N.of A	77.0000	O: Density	2.8000
Val.A	6.0000	O: Melt.temp.	2820.0000
M.N.ofB	101.0000		
Val.B	2.0000		
M.N.of A	73.0000	O: Density	3.5400
Val.A	6.0000	O: Melt.temp.	3080.0000
M.N.ofB	101.0000		
Val.B	2.0000		
M.N.of A	76.0000	O: Density	5.6700
Val.A	6.0000	O: Melt.temp.	2253.0000
M.N.ofB	101.0000		
Val.B	2.0000		
M.N.of A	16.0000	O: Density	3.3200
Val.A	6.0000	O: Melt.temp.	2887.0000
M.N.ofB	101.0000		
Val.B	2.0000		
M.N.of A	15.0000	O: Density	4.2000
Val.A	6.0000	O: Melt.temp.	2727.0000
M.N.ofB	101.0000		
Val.B	2.0000		
M.N.of A	14.0000	O: Density	5.7600
Val.A	6.0000	O: Melt.temp.	2196.0000
M.N.ofB	101.0000		
Val.B	2.0000		

M.N.of A	51.0000	O: Density	4.9300
Val.A	4.0000	O: Melt.temp.	1263.0000
M.N.ofB	101.0000		
Val.B	2.0000		

M.N.of A	54.0000	O: Density	5.2300
Val.A	3.0000	O: Melt.temp.	2322.0000
M.N.ofB	101.0000		
Val.B	2.0000		

M.N.of A	53.0000	O: Density	2.8000
Val.A	3.0000	O: Melt.temp.	2218.0000
M.N.ofB	101.0000		
Val.B	2.0000		

M.N.of A	51.0000	O: Density	5.4400
Val.A	4.0000	O: Melt.temp.	3223.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	49.0000	O: Density	7.3500
Val.A	4.0000	O: Melt.temp.	3253.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	50.0000	O: Density	13.9000
Val.A	4.0000	O: Melt.temp.	3660.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	54.0000	O: Density	6.0200
Val.A	3.0000	O: Melt.temp.	2450.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	53.0000	O: Density	8.3600
Val.A	3.0000	O: Melt.temp.	2477.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	52.0000	O: Density	14.3600
Val.A	3.0000	O: Melt.temp.	3366.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	57.0000	O: Density	6.1400
Val.A	2.0000	O: Melt.temp.	1772.0000
M.N.ofB	100.0000		
Val.B	3.0000		

M.N.of A	56.0000	O: Density	9.1800
Val.A	2.0000	O: Melt.temp.	1172.0000
M.N.ofB	100.0000		
Val.B	3.0000		

| M.N.of A | 55.0000 | O: Density | 12.1000 |

Val.A	2.0000	O: Melt.temp.	873.0000
M.N.ofB	100.0000		
Val.B	3.0000		
M.N.of A	54.0000	O: Density	6.6898
Val.A	3.0000	O: Melt.temp.	2311.3718
M.N ofB	100.0000		
Val.B	3.0000		
M.N.of A	53.0000	O: Density	8.6104
Val.A	3.0000	O: Melt.temp.	2606.4585
M.N.ofB	100.0000		
Val.B	3.0000		
M.N.of A	52.0000	O: Density	13.8339
Val A	3.0000	O: Melt.temp.	3444.5763
M.N.ofB	100.0000		
Val.B	3.0000		

Val.A	2.0000	O: Melt.temp.	873.0000

Chapter 6

Conclusions and Future Work

6.1 Conclusions

This work is about trends in material data for binary ceramic compounds. The major aspects can be summed up as follows:

1. A database comprising of property data for about 60 ceramic compounds has been developed.

2. The compiled data has been used to determine property ranges and to explore various correlations.

3. Property ranges for various categories of materials including ceramics are compared which are useful for materials selection in mechanical design.

4. Correlations between various physical properties are discussed and the limits

of correlations are described for ceramic compounds. Based on above correlation ,estimates are made for a few compound and compared with literature value.

5. Neural Networks are developed for estimating various properties. After querring these networks, a good comparative values of the properties are obtained for materials. The concept of "informed neural network" was applied and it was found that it yields better estimates.

6. Neural Networks are developed for Borides, nitrides, carbides and oxides using Mendeleev number and valency as input a good estimate of melting point and density is made.

Preliminary results support the hypothesis that since Mendeleev number allows good structural separation of compounds in Pettifor maps, it should also be useful index in developing correlations with various properties of refractory compounds.

6.2 Suggestions for Future work

The present work is a first attempt to develop correlations between properties of materials based on various approaches including structure maps, and neural networks. Although the results are encouraging the work should be extended to cover more compounds and properties. It would then be possible to ascertain the utility as well as to carry out a comparative evaluation of these approaches.

References

1   P. William Lee, *Ceramics.*, Reinhold Publishing Corporation, 1961

2   W.D. Kingrey, *Introduction to Ceramics,* John Wiley and Sons, 1965

3   David W. Richerson, *Modern Ceramic Engineering,*1982,p376-392

4   *Ullmann's Encyclopedia of Industrial Chemistry* edited by Wolfgang
    Gerhartz,Y. Stephen Yamamoto, Thomas Campbell, Rudolf Pfefferkorn, James
    F. Rounsaville,vA4, 1985, p296-306

5   *Ullmann's Encyclopedia of Industrial Chemistry* edited by Wolfgang
    Gerhartz,Y. Stephen Yamamoto, Thomas Campbell, Rudolf Pfefferkorn, James F.
    Rounsaville,vA5, 1986, p61-77

6   *Ullmann's Encyclopedia of Industrial Chemistry* edited by Barbara Elvers,
    Stephen Hawkins, Gail Shulz,vA17,1991, p341-357

7   Eugene Ryshkewitch, *Oxide Ceramics* ,Academic press, 1972, p109-388

8   *Checks and Estimates for Material Properties,* M.F.Ashby, Cambrige Engg.
    Design center, 1996

9   P. Villars , *J. less- Comma Met.,*92,1983, 215

10 P. Villars, *J.less- Comma Met.,*99,1984,33

11 P.Villers,*J.less- Comma Met.,*102, 1985, 199

12 W.B. Pearson, *The Crystal Chemistry and Physics of Metals and Alloys,* John
    Wiley and Sons, New York, 1972

13 D.G. Pettifer,*First supplement to the Pergomon Encyclopedia of Materials
    Science and Engineering,* edited by R.W. Cahn, Pergamon, Oxford, 1988,p51

14 D.G. Pettifer , *New Sci.,*110, (1510), 1986

15 D.G. Pettifer , *Physical Metallurgy,* edited by R.W. Cahn and P.Haasen, chapter
    3, 73-152, 1983, Amsterdam, North-Holland, 1983

16 D.G. Pettifer, *J. Phys. C,* Solid State Phys.,19,1986, 285

17 D.G. Pettifer and R.Podloucky, *Phys. Rev. Lett.,*55, 1985, 261

18 D.G. Pettifer, *Mat. Sc. And Tech.,* 4,1988, 675

19 M.F. Ashby and David R.H.Jones, *Engineering Materials: An Introduction to their properties and applications*, **v34**, Pergamon Press, 1980

20 Priyanka awasthi,Om Prakash ,*Materials property data for binary ceramic compounds*, IITK-ME-M&D-TR05, Department of mechanical engineering, Indian Institute of Technology, Kanpur, India, May 2001

21 D. R. Askeland, *The Science and Engineering of Materials*, Chapman and Hall 1990

22 *CRC handbook of Chemistry & Physics*, 79th ed, edited by David R.Lide,CSC Press LLC, 1998

23 M.F. Ashby, *Material Selection in Mechanical Design*, 2nd edn, Butterworth-Heinemann, 1992

24 Touloukian , *Thermo physical properties of materr: Thermal conductivity of metallic element and alloys* , The TPRC data series,**v1**, 1970

25 Touloukian,*Thermo physical properties of matter : Thermal expansion of metals and alloys*, The TPRC data series,**v12**, 1975

26 Smith ,*Metals Reference Book*, 6th edn., edited by Eric A. Brandes,   R669 Sm6m6

27 Intermetallic *Compounds: Principles & Practice*, edited by J.H. Westbrook and R.L. Fleischer, **v1**, John Wiley & Sons, 1995

28 F.Ashby, *Engineering Material: An Introduction to microstructures, Processing and Design*,**v39**, Pergamon Press, 1986

29 B. Chalmers, *Physical metallurgy*, John Wiley& sons, 1962

30 W.B.Pearson , *Handbook of lattice spacings, structure of metals and alloys*, Pergamon Press, 1967

31 W.F.Pearson , *Handbook of lattice spacings, structure of metals and alloys* Pergamon Press, 1958

32 *Encyclopedia of Material Science & Engineering* ,**v1**, edited by R.Cahn, Pergamon Press, 1998

33 *Rules of Thumb for physical scientists*, compiled by D.J. Fisher, Trans Tech publications Ltd., Switzerland, 1998.

34 P. Paufler, *intermetallic phasen* VEB Deutscher Verlag furGrundstoffindustrie Leipzig, 1976,165

35 R.L. Fleischer,*Proc. Int. Symp. Intermetallic Compounds* edited by O. Izumi, The Japan Institute of Metals, Sendai, 1991a, 157

36 A.A. Ivanko,*Handbook of Hardness Data,* edited by G.V. Samsonov, Akad.Sci. Ukranian SSSR, 1971

37 R.L. Fleischer, R.S. Gilmore and R.J. Zabala, *J. Appl. Phys.*,64, 1988,2964

38 R.L. Fleischer, R.S. Gilmore and R.J. Zabala, *Acta. Meta.*,37, 1989, 2801

39 Jacek M. Zurada ,*Introduction to Artificial Neural Systems* Jaico Publishing House , 1999

40 *Crystallographic data on metal and alloy Structures* compiled by A.Taylor and Brenda J. Kagle , Mills Memorial Library,1962

41 *Intermetallic compounds, Principle and Practice,* edited by J.H. Westbrook and R.L. Fischer,v2 John Wiley & sons ,1995, p12

42 *Intermetallic compounds Principle and Practice,* edited by J.H. Westbrook And R.L.Fischer , v2 John Wiley & sons, 1995,p 269

43 *Materials data compilation* by M.F.Ashby and   A.M . Brown , Cambridge University, 1980

44 *CRC Materials Science and Engineering Handbook,* 2nd ed.,   edited by James F. Shackelford , William Alexander , Jun S. Park , 1994, p259-345

45 1987 IEEE, ASSP Lipman R. *An introduction   to computing with   neural networks,* p 4-18

46 H.K.D.H. Bhadeshia, ISIJ International ,v39, 1999, p966-979

47 © 1999-2000 Stephen Wolestenholme , http://www. uksharereg.com/easynn.html

48 D.J.C. McKay Neural Computation, v4, 1992, p415-472.

49 Om Prakash, *Informed neural networks for prediction of materials propertry data ,* IITK-ME-M&D-TR03, Department of mechanical engineering,   Indian Institute of Technology, Kanpur, India, July 2000

Crystal Structure of Binary Compounds

The crystal structures of tens of thousands of binary, ternary and quaternary phases have been developed since the advent of x-ray crystallography in 1910. These crystal structures are having importance in alloy formation. In this section we will see various nomenclatures which describe the crystal structures of various materials In the following section we will see in brief about crystal structure of refractory compounds.

A.1 Crystal structure nomenclature

In general crystals structures are preliminarily classified according to the fourteen Bravais lattices and then the number of atoms in the conventional crystallographic Unit cell for standard space group. Secondary classification within these groups follows the numerical order of 230 space groups and finally within any space group structures follow an alphabetical order of their names. The important nomenclatures that generally come across are given below

- ASTM nomenclature
- Pearson nomenclature
- Strukturbericht type

ASTM nomenclature

ASTM uses a single arbitrary capital letter to characterize each of fourteen Bravais lattice as shown in Table A.1.

Pearson nomenclature

Pearson chosen two characters, which are widely used to identify crystal types The nomenclature involves a small letter to identify the space lattice.He retained the crystallographic letters for this purpose. To these is added a number equal to the number of atoms in the unit cell conventionally selected for a particular crystal type. When determining number of atoms in the unit cell, it should be remembered that each atom that is shared with an adjacent cell (or cells) must be counted as only a fraction of an atom The Pearson symbols for the fourteen space lattices are shown in Table A.1

Strukturbericht type

There are indefinite number of structural types falling under a given class.

Table A.1: Representative nomenclatures for fourteen Bravais lattices

Crystal System	Lattice Parameters & Angles	Space lattice	Lattice symbol	Small letter designation by Pearson	Pearson Symbol	ASTM symbol
Triclinic (anorthic)	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	Primitive	P	a	aP	Z
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$ or $a \neq b \neq c$ $\alpha = \beta = 90 \neq \gamma$	Primitive Base – centered	P C	m	mP mC	M N
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive Base – centered Face – centered Body – centered	P C F I	o	oP oC oF oI	O Q S P
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive Body – centered	P I	t	tP tI	T U
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	Primitive	P	h	hP	H
Rhombohedral (or trigonal)	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$ $<120^\circ$	Primitive	R	h	hR	R
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive Face – centered Body – centered	P F I	c	cP cF cI	C F B

symbols, space groups , structure prototypes and Strukturbericht designations for crystal structures are shown in Table A.2

A.3 Crystal structure of Ceramic Compounds

Refractory compounds have different crystal structure of its constituent chemical elements in the binary case or of its binary boundary refractory compounds in the ternary case. A crystal structure is completely determined by the following data.

- Chemical formula
- Crystal system and unit cell dimensions
- Space group
- Occupation number and coordinates of the occupied point sets

The first crystal studies of refractory compounds showed relatively simple structures like those of common metals. Hundreds of crystallographic analysis have been completed. It is apparent that this group of compounds embraces many exceeding complex structural arrangements. The most common structures are among the most simple, certain of these belongings to the AB, AB_2 and AB_3 types.

Some example of these structures are shown in Fig.A.1.

AB
TYPES

Na Cl

Cs Cl

Zn S
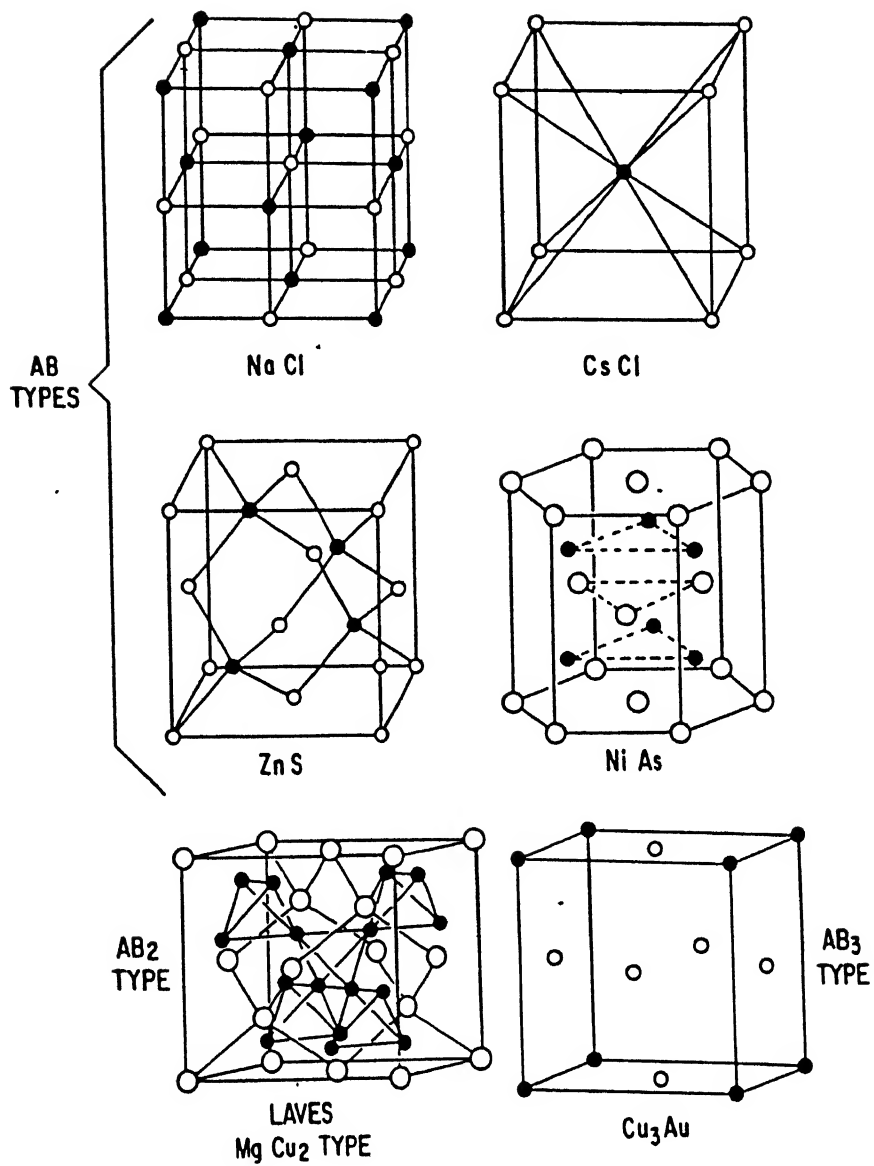
Ni As

AB₂
TYPE

LAVES
Mg Cu₂ TYPE

AB₃
TYPE

Cu₃Au

Fig A.1: Some examples of crystal structure

Crystal Structure Nomenclature*

Arranged Alphabetically by Pearson-Symbol Designation

Pearson symbol	Prototype	Strukturbericht designation	Space group	Pearson symbol	Prototype	Strukturbericht designation	Space group
cF4	Cu	$A1$	$Fm\bar{3}m$	cP6	Ag_2O	$C3$	$Pn\bar{3}m$
cF8	C (diamond)	$A4$	$Fd\bar{3}m$	cP7	CaB_6	$D2_1$	$Pm\bar{3}m$
	NaCl (rock salt)	$B1$	$Fm\bar{3}m$	cP8	Cr_3Si (βW)	$A15$	$Pm\bar{3}n$
	ZnS (sphalerite)	$B3$	$F\bar{4}3m$		FeSi	$B20$	$P2_13$
cF12	CaF_2 (fluorite)	$C1$	$Fm\bar{3}m$		Cu_3VS_4 (sulvanite)	$H2_4$	$P\bar{4}3m$
	MgAgAs	$C1_b$	$F\bar{4}3m$	cP12	FeS_2 (pyrite)	$C2$	$Pa3$
cF16	$AlCu_2Mn$ (Heusler)	$L2_1$	$Fm\bar{3}m$		NiSbS (ullmanite)	$F0_1$	$P2_13$
	BiF_3 ($AlFe_3$)	DO_3	$Fm\bar{3}m$		βMn	$A13$	$P4_132$
	NaTl	$B32$	$Fd\bar{3}m$	cP20	$BaHg_{11}$	$D2_e$	$Pm\bar{3}m$
cF24	$AuBe_5$	$C15_b$	$F\bar{4}3m$	cP36	Mg_2Zn_{11}	$D8_c$	$Pm\bar{3}$
	SiO_2 (β cristobalite)	$C9$	$Fd\bar{3}m$	cP39	Cu_9Al_4 (γ brass)	$D8_3$	$P\bar{4}3m$
	Cu_2Mg (Laves)	$C15$	$Fd\bar{3}m$	cP52	$HgSn_{6\text{-}10}$	A_f	$P6/mmm$
cF32	$CuPt_3$	$L1_1$	$Fm\bar{3}c$	hP1	Mg	$A3$	$P6_3/mmc$
cF52	UB_{12}	$D2_f$	$Fm\bar{3}m$	hP2	WC	B_h	$P\bar{6}m2$
cF56	Al_2MgO_4 (spinel)	$H1_1$	$Fd\bar{3}m$		AlB_2	$C32$	$P6/mmm$
	Co_3S_4	$D7_2$	$Fd\bar{3}m$	hP3	CdI_2	$C6$	$P\bar{3}m1$
cF68	Co_9S_8	$D8_9$	$Fm\bar{3}m$		Fe_2N	$L'3$	$P6_3/mmc$
cF80	Sb_2O_3 (senarmontite)	$D5_4$	$Fd\bar{3}m$		$LiZn_2$	C_k	$P6_3/mmc$
cF112	Fe_3W_3C (η carbide)	$E9_3$	$Fd\bar{3}m$		γSe	$A8$	$P3_121$
	$NaZn_{13}$	$D2_3$	$Fm\bar{3}c$	hP4	αLa	$A3'$	$P6_3/mmc$
cF116	$Cr_{23}C_6$	$D8_4$	$Fm\bar{3}m$		BN	B_k	$P6_3/mmc$
	$Mn_{23}Th_6$, $Cu_{16}Mg_6Si_7$ (G-phase)	$D8_4$	$Fm\bar{3}m$		C (graphite)	$A9$	$P6_3/mmc$
cI2	W	$A2$	$Im\bar{3}m$		NiAs	$B8_1$	$P6_3/mmc$
cI16	CoU	B_e	$I2_13$		ZnS (wurtzite)	$B4$	$P6_3mc$
cI28	Th_3P_4	$D7_3$	$I\bar{4}3d$	hP5	La_2O_3	$D5_2$	$P\bar{3}m1$
cI32	$CoAs_3$ (skutterudite)	DO_2	$Im\bar{3}$		Ni_2Al_3	$D5_{13}$	$P\bar{3}m1$
cI40	Ge_7Ir_3	$D8_f$	$Im\bar{3}m$	hP6	$CaCu_5$	$D2_d$	$P6/mmm$
	Pu_2C_3	$D5_c$	$I\bar{4}3d$		CoSn	$B35$	$P6/mmm$
cI52	Cu_5Zn_8 (γ brass)	$D8_2$	$I\bar{4}3m$		Cu_2Te	C_h	$P6/mmm$
	Fe_3Zn_{10} (γ brass)	$D8_1$	$Im\bar{3}m$		HgS	$B9$	$P3_121$
cI54	Sb_2Tl_7	$L2_2$	$Im\bar{3}m$		MoS_2	$C7$	$P6_3/mmc$
cI58	αMn (χ-phase)	$A12$	$I\bar{4}3m$		Ni_2In	$B8_2$	$P6_3/mmc$
cI76	$Cu_{15}Si_4$	$D8_6$	$I\bar{4}3d$	hP8	Na_3As	DO_{18}	$P6_3/mmc$
cI80	Mn_2O_3	$D5_3$	$Ia\bar{3}$		Ni_3Sn	DO_{19}	$P6_3/mmc$
cI96	$AlLi_3N_2$	$E9_d$	$Ia\bar{3}$		TiAs	B_i	$P6_3/mmc$
cI162	$Mg_{32}(Al,Zn)_{49}$	$D8_e$	$Im\bar{3}$	hP9	$CrSi_2$	$C40$	$P6_222$
cP1	αPo	A_h	$Pm\bar{3}m$		Fe_2P	$C22$	$P\bar{6}2m$
cP2	CsCl	$B2$	$Pm\bar{3}m$		ζAgZn	B_b	$P\bar{3}$
cP4	$AuCu_3$	$L1_2$	$Pm\bar{3}m$		SiO_2 (high quartz)	$C8$	$P6_222$
	ReO_3	DO_9	$Pm\bar{3}m$	hP10	Pt_2Sn_3	$D5_b$	$P6_3/mmc$
cP5	$AlFe_3C$ (perovskite)	$L'1_2$	$Pm\bar{3}m$	hP12	CuS	$B18$	$P6_3/mmc$
	$CaTiO_3$ (perovskite)	$E2_1$	$Pm\bar{3}m$		$MgZn_2$ (Laves)	$C14$	$P6_3/mmc$
	Fe_4N	$L'1$	$P\bar{4}3m$		SiO_2 (β tridymite)	$C10$	$P6_3/mmc$

Table A.2: Crystal structure nomenclatures are arranged alphabetically by Pearson symbol designation and Strukturbericht designation

Pearson symbol	Prototype	Strukturbericht designation	Space group
4	W₂B₅	$D8_h$	$P6_3/mmc$
6	Mn₅Si₃	$D8_8$	$P6_3/mcm$
18	Ni₃Ti	$D0_{24}$	$P6_3/mmc$
	Al₄C₄Si	$E9_4$	$P6_3mc$
	Al₈FeMg₃Si₆	$E9_b$	$P\bar{6}2m$
	Mg₂Ni	C_a	$P6_222$
20	Fe₃Th₇	$D10_2$	$P6_3mc$
	Th₇S₁₂	$D8_k$	$P6_3/m$
24	Cu₃P	$D0_{21}$	$P6_3cm$
	MgNi₂ (Laves)	$C36$	$P6_3/mmc$
28	Co₂Al₅	$D8_{11}$	$P6_3/mmc$
1	αHg	$A10$	$R\bar{3}m$
	βPo	A_i	$R\bar{3}m$
2	αAs	$A7$	$R\bar{3}m$
3	αSm	$C19$	$R\bar{3}m$
4	NaCrS₂	$F5_1$	$R\bar{3}m$
5	Bi₂Te₃	$C33$	$R\bar{3}m$
	Ni₃S₂	$D5_e$	$R32$
6	CaSi₂	$C12$	$R\bar{3}m$
	NiS (millerite)	$B13$	$R\bar{3}m$
7	Al₄C₃	$D7_1$	$R\bar{3}m$
	Mo₂B₅	$D8_i$	$R\bar{3}m$
10	αAl₂O₃ (corundum)	$D5_1$	$R\bar{3}c$
13	Fe₇W₆ (μ-phase)	$D8_5$	$R\bar{3}m$
15	B₄C	$D1_g$	$R\bar{3}m$
26	Cr₅Al₈	$D8_{10}$	$R\bar{3}m$
32	CuPt	$L1_1$	$R\bar{3}m$
C6	AuTe₂ (calaverite)	$C34$	$C2/m$
C8	CuO (tenorite)	$B26$	$C2/c$
C12	ThC₂	C_g	$C2/c$
C14	δNi₃Sn₄	$D7_a$	$C2/m$
C16	FeKS₂	$F5_a$	$C2/c$
P12	AgAuTe₄ (sylvanite)	$E1_b$	$P2/c$
	ZrO₂	$C43$	$P2_1/c$
P20	As₂S₃	$D5_f$	$P2_1/c$
P22	Co₂Al₉	$D8_d$	$P2_1/c$
P24	FeAsS	$E0_7$	$P2_1/c$
P32	AsS (realgar)	B_f	$P2_1/c$
	βSe	A_i	$P2_1/c$
P64	αSe	A_k	$P2_1/c$
C4	αU	$A20$	$Cmcm$
C8	CaSi	B_c	$Cmmc$
	αGa	$A11$	$Cmca$
	CrB	$B33$	$Cmcm$
	I₂	$A14$	$Cmca$
	P (black)	$A17$	$Cmca$
C12	ZrSi₂	$C49$	$Cmcm$
C16	BRe₃	$E1_a$	$Cmcm$
C20	PdSn₄	$D1_c$	$Aba2$
C24	PdSn₂	C_e	$Aba2$
C28	Al₆Mn	$D2_h$	$Cmcm$
F24	TiSi₂	$C54$	$Fddd$
F40	Mn₄B	$D1_f$	$Fddd$
F48	CuMg₂	C_b	$Fddd$
F72	GeS₂	$C44$	$Fdd2$
F128	αS	$A16$	$Fddd$
I12	SiS₂	$C42$	$Ibam$
I14	Ta₃B₄	$D7_b$	$Immm$
I20	Al₃U	$D1_b$	$Imma$
I28	Ga₂Mg₅	$D8_f$	$Ibam$
	As₂C₃	$B19$	$Pmma$
oP8	βCu₃Ti	$D0_a$	$Pmmn$
	FeB	$B27$	$Pnma$
	GeS	$B16$	$Pnma$
	SnS	$B29$	$Pmcn$
	MnP	$B31$	$Pnma$
	TiB	B_m	$Pnma$
oP12	Co₂Si, NiSiTi (E-phase)	$C23$	$Pnma$
	Co₂Si	$C37$	$Pbnm$
	HgCl₂	$C28$	$Pmnb$
oP16	Al₃Ni	$D0_{20}$	$Pnma$
	AsMn₃	$D0_d$	$Pmmn$
	BaS₃	$D0_{17}$	$P42_1m$
	CdSb	B_e	$Pbca$
	CuS₂Sb (wolfsbergite)	$F5_6$	$Pnma$
	Fe₃C (cementite)	$D0_{11}$	$Pnma$
oP20	Cr₃C₂	$D5_{10}$	$Pnma$
	Sb₂S₃	$D5_8$	$Pnma$
	Sb₂O₃ (valentinite)	$D5_{11}$	$Pccn$
oP24	AuTe₂ (krennerite)	$C46$	$Pma2$
	CuFe₂S₃ (cubanite)	$E9_i$	$Pnma$
	TiO₂ (brookite)	$C21$	$Pbca$
oP40	Cr₇C₃	$D10_1$	$Pnma$
tI2	αPa	A_a	$I4/mmm$
	In	$A6$	$I4/mmm$
tI4	βSn	$A5$	$I4_1/amd$
tI6	CaC₂	$C11_a$	$I4/mmm$
	MoSi₂	$C11_b$	$I4/mmm$
	ThI₂	$L'2_b$	$I4/mmm$
tI8	Al₃Ti	$D0_{22}$	$I4/mmm$
	Al₄Ba	$D1_3$	$I4/mmm$
	MoNi₄	$D1_a$	$I4/m$
tI12	Al₂Cu	$C16$	$I4/mcm$
	ThSi₂	C_c	$I4_1/amd$
tI14	Al₂CdS₄	$E3$	$I\bar{4}$
tI16	Al₃Zr	$D0_{23}$	$I4/mmm$
	CuFeS₂ (chalcopyrite)	$E1_1$	$I\bar{4}2d$
	Cu₂FeSnS₄ (stannite)	$H2_6$	$I\bar{4}2m$
	Ir₃Si	$D0_c'$	$I4/mcm$
	MoB	B_g	$I4_1/amd$
	SiU₃	$D0_c$	$I4/mcm$
	TlSe	$B37$	$I4/mcm$
tI18	Fe₈N	$D2_g$	$I4/mmm$
tI26	Mn₁₂Th	$D2_b$	$I4/mmm$
tI28	MnU₆	$D2_c$	$I4/mcm$
tI32	Cr₅B₃	$D8_l$	$I4/mcm$
	Ni₃P	$D0_e$	$I\bar{4}$
	W₅Si₃	$D8_m$	$I4/mcm$
tP2	δCuTi	$L2_a$	$P4/mmm$
tP4	βNp	A_d	$P42_12$
	AuCu	$L1_0$	$P4/mmm$
	CuTi₃	$L6_0$	$P4/mmm$
	γCuTi	$B11$	$P4/nmm$
	PbO	$B10$	$P4/nmm$
	PtS	$B17$	$P4_2/mmc$
tP6	Cu₂Sb	$C38$	$P4/nmm$
	PbFCl	$E0_1$	$P4/nmm$
	TiO₂ (rutile)	$C4$	$P4_2/mnm$
tP10	Pb₄Pt	$D1_d$	$P4/nbm$
	Si₂U₃	$D5_a$	$P4/mbm$
tP16	PdS	$B34$	$P4_2/m$
tP20	B₄Th	$D1_e$	$P4/mbm$
tP30	βU	A_b	$P4_2/mnm$

Strukturbericht designation	Prototype	Pearson symbol	Space group
	αPa	$tI2$	$I4/mmm$
	βU	$tP30$	$P4_2/mnm$
	αNp	$oP8$	$Pnmu$
	βNp	$tP4$	$P42_12$
	HgSn$_{6-10}$	$hP1$	$P6/mmm$
	γB	$tP50$	$P4_2/nnm$
	αPo	$cP1$	$Pm\bar{3}m$
	βPo	$hR1$	$R\bar{3}m$
	αSe	$mP64$	$P2_1/c$
	βSe	$mP32$	$P2_1/c$
	Cu	$cF4$	$Fm\bar{3}m$
	W	$CI2$	$Im\bar{3}m$
	Mg	$hP2$	$P6_3/mmc$
	αLa	$hP4$	$P6_3/mmc$
	C (diamond)	$cF8$	$Fd\bar{3}m$
	βSn	$tI4$	$I4_1/amd$
	In	$tI2$	$I4/mmm$
	αAs	$hR2$	$R\bar{3}m$
	γSe	$hP3$	$P3_121$
	C (graphite)	$hP4$	$P6_3/mmc$
	αHg	$hR1$	$R\bar{3}m$
	αGa	$oC8$	$Cmca$
	αMn (χ-phase)	$cI58$	$I\bar{4}3m$
	βMn	$cP20$	$P4_132$
	I$_2$	$oC8$	$Cmca$
	Cr$_3$Si (β-W)	$cP8$	$Pm\bar{3}n$
	αS	$oF128$	$Fddd$
	P (black)	$oC8$	$Cmca$
	αU	$oC4$	$Cmcm$
	CoU	$cI16$	$I2_13$
	ʃAgZn	$hP9$	$P\bar{3}$
	CaSi	$oC8$	$Cmmc$
	ηNiSi	$oP8$	$Pbnm$
	CdSb	$oP16$	$Pbca$
(B33)	CrB	$oC8$	$Cmcm$
	MoB	$tI16$	$I4_1/amd$
	WC	$hP2$	$P\bar{6}m2$
	TiAs	$hP8$	$P6_3/mmc$
	BN	$hP4$	$P6_3/mmc$
	AsS (realgar)	$mP32$	$P2_1/c$
	TiB	$oP8$	$Pnma$
	NaCl (rock salt)	$cF8$	$Fm\bar{3}m$
	CsCl	$cP2$	$Pm\bar{3}m$
	ZnS (sphalerite)	$cF8$	$F\bar{4}3m$
	ZnS (wurtzite)	$hP4$	$P6_3mc$
	NiAs	$hP4$	$P6_3mmc$
	Ni$_2$In	$hP6$	$P6_3mmc$
	HgS (cinnabar)	$hP6$	$P3_121$
	PbO	$tP4$	$P4/nmm$
	γCuTi	$tP4$	$P4/nmm$
	NiS (millerite)	$hR6$	$R\bar{3}m$
	GeS	$oP8$	$Pnma$
	PtS (cooperite)	$tP4$	$P4_2/mmc$
	CuS (covelite)	$hP12$	$P6_3/mmc$
	AuCd	$oP4$	$Pmma$

| Strukturbericht designation	Prototype	Pearson symbol	Space group
B20	FeSi	$cP8$	$P2_13$
B26	CuO (tenorite)	$mC8$	$C2/c$
B27	FeB	$oP8$	$Pnma$
B29	SnS	$oP8$	$Pmcn$
B31	MnP	$oP8$	$Pnma$
B32	NaTl	$cF16$	$Fd\bar{3}m$
B33$(=B_f)$	CrB	$oC8$	$Cmcm$
B34	PdS	$tP16$	$P4_2/m$
B35	CoSn	$hP6$	$P6/mmm$
B37	TlSe	$tI16$	$I4/mcm$
C_a	Mg$_2$Ni	$hP18$	$P6_222$
C_b	CuMg$_2$	$oF48$	$Fddd$
C_c	ThSi$_2$	$tI12$	$I4_1/amd$
C_e	PdSn$_2$	$oC24$	$Aba2$
C_g	ThC$_2$	$mC12$	$C2/c$
C_h	Cu$_2$Te	$hP6$	$P6/mmm$
C_k	LiZn$_2$	$hP3$	$P6_3/mmc$
C1	CaF$_2$ (fluorite)	$cF12$	$Fm\bar{3}m$
C1$_b$	MgAgAs	$cF12$	$F\bar{4}3m$
C2	FeS$_2$ (pyrite)	$cP12$	$Pa3$
C3	Ag$_2$O	$cP6$	$Pn\bar{3}m$
C4	TiO$_2$ (rutile)	$tP6$	$P4_2/mnm$
C6	CdI$_2$	$hP3$	$P\bar{3}m1$
C7	MoS$_2$	$hP6$	$P6_3/mmc$
C8	SiO$_2$ (high quartz)	$hP9$	$P6_222$
C9	SiO$_2$ (β cristobalite)	$cF24$	$Fd3m$
C10	SiO$_2$ (β tridymite)	$hP12$	$P6_3/mmc$
C11$_a$	CaC$_2$	$tI6$	$I4/mmm$
C11$_b$	MoSi$_2$	$tI6$	$I4/mmm$
C12	CaSi$_2$	$hR6$	$R\bar{3}m$
C14	MgZn$_2$ } Laves	$hP12$	$P6_3/mmc$
C15	Cu$_2$Mg }	$cF24$	$Fd\bar{3}m$
C15$_b$	AuBe$_5$	$cF24$	$F\bar{4}3m$
C16	Al$_2$Cu	$tI12$	$I4/mcm$
C18	FeS$_2$ (marcasite)	$oP6$	$Pnnm$
C19	αSm	$hR3$	$R\bar{3}m$
C21	TiO$_2$ (brookite)	$oP24$	$Pbca$
C22	Fe$_2$P	$hP9$	$P\bar{6}2m$
C23	Co$_2$Si, NiSiTi (E-phase)	$oP12$	$Pnma$
C28	HgCl$_2$	$oP12$	$Pmnb$
C32	AlB$_2$	$hP3$	$P6/mmm$
C33	Bi$_2$Te$_3$	$hR5$	$R\bar{3}m$
C34	AuTe$_2$ (calaverite)	$mC6$	$C2/m$
C35	CaCl$_2$	$oP6$	$Pnnm$
C36	MgNi$_2$ (Laves)	$hP24$	$P6_3/mmc$
C37	Co$_2$Si	$oP12$	$Pbnm$
C38	Cu$_2$Sb	$tP6$	$P4/nmm$
C40	CrSi$_2$	$hP9$	$P6_222$
C42	SiS$_2$	$oI12$	$Ibam$
C43	ZrO$_2$	$mP12$	$P2_1/c$
C44	GeS$_2$	$oF72$	$Fdd2$
C46	AuTe$_2$ (krennerite)	$oP24$	$Pma2$
C49	ZrSi$_2$	$oC12$	$Cmcm$
C54	TiSi$_2$	$oF24$	$Fddd$
D0$_a$	βCu$_3$Ti	$oP8$	$Pmmn$
D0$_c$	SiU$_3$	$tI16$	$I4/mcm$

continued

Arranged Alphabetically by Strukturbericht Designation (*continued*)

Strukturbericht designation	Prototype	Pearson symbol	Space group	Strukturbericht designation	Prototype	Pearson symbol	Space group
$D0'_c$	Ir_3Si	$tI16$	$I4/mcm$	$D8_d$	Co_2Al_9	$mP22$	$P2_1/c$
$D0_d$	$AsMn_3$	$oP16$	$Pmmn$	$D8_e$	$Mg_{32}(Al,Zn)_{49}$	$cI162$	$Im\bar{3}$
$D0_e$	Ni_3P	$tI32$	$I\bar{4}$	$D8_f$	Ge_7Ir_3	$cI40$	$Im\bar{3}m$
$D0_2$	$CoAs_3$ (skutterudite)	$cI32$	$Im\bar{3}$	$D8_g$	Ga_2Mg_5	$oI28$	$Ibam$
$D0_3$	$BiF_3, AlFe_3$	$cF16$	$Fm\bar{3}m$	$D8_h$	W_2B_5	$hP14$	$P6_3/mmc$
$D0_9$	ReO_3	$cP4$	$Pm\bar{3}m$	$D8_i$	Mo_2B_5	$hR7$	$R\bar{3}m$
$D0_{11}$	Fe_3C (cementite)	$oP16$	$Pnma$	$D8_k$	Th_7S_{12}	$hP20$	$P6_3/m$
$D0_{17}$	BaS_3	$oP16$	$P42_1m$	$D8_l$	Cr_5B_3	$tI32$	$I4/mcm$
$D0_{18}$	Na_3As	$hP8$	$P6_3/mmc$	$D8_m$	W_5Si_3	$tI32$	$I4/mcm$
$D0_{19}$	Ni_3Sn	$hP8$	$P6_3/mmc$	$D8_1$	Fe_3Zn_{10}	$cI52$	$Im\bar{3}m$
$D0_{20}$	Al_3Ni	$oP16$	$Pnma$	$D8_2$	Cu_5Zn_8 $\}$ γ brass	$cI52$	$I\bar{4}3m$
$D0_{21}$	Cu_3P	$hP24$	$P6_3cm$	$D8_3$	Cu_9Al_4	$cP52$	$P\bar{4}3m$
$D0_{22}$	Al_3Ti	$tI8$	$I4/mmm$	$D8_4$	$Cr_{23}C_6$	$cF116$	$Fm\bar{3}m$
$D0_{23}$	Al_3Zr	$tI16$	$I4/mmm$	$D8_5$	Fe_7W_6 (μ-phase)	$hR13$	$R\bar{3}m$
$D0_{24}$	Ni_3Ti	$hP16$	$P6_3/mmc$	$D8_6$	$Cu_{15}Si_4$	$cI76$	$I\bar{4}3d$
$D1_a$	$MoNi_4$	$tI10$	$I4/m$	$D8_8$	Mn_5Si_3	$hP16$	$P6_3/mcm$
$D1_b$	Al_4U	$oI20$	$Imma$	$D8_9$	Co_9S_8	$cF68$	$Fm\bar{3}m$
$D1_c$	$PdSn_4$	$oC20$	$Aba2$	$D8_{10}$	Cr_5Al_8	$hR26$	$R\bar{3}m$
$D1_d$	Pb_4Pt	$tP10$	$P4/nbm$	$D8_{11}$	Co_2Al_5	$hP28$	$P6_3/mmc$
$D1_e$	B_4Th	$tP20$	$P4/mbm$	$D10_1$	Cr_7C_3	$oP40$	$Pnma$
$D1_f$	Mn_4B	$oF40$	$Fddd$	$D10_2$	Fe_3Th_7	$hP20$	$P6_3mc$
$D1_g$	B_4C	$hR15$	$R\bar{3}m$	$D8_{11}$	Co_2Al_5	$hP28$	$P6_3/mmc$
$D1_3$	Al_4Ba	$tI10$	$I4/mmm$	$E0_1$	$PbFCl$	$tP6$	$P4/nmm$
$D2_b$	$Mn_{12}Th$	$tI26$	$I4/mmm$	$E0_7$	$FeAsS$	$mP24$	$P2_1/c$
$D2_c$	MnU_6	$tI28$	$I4/mcm$	$E1_a$	$MgCuAl_2$	$oC16$	$Cmcm$
$D2_d$	$CaCu_5$	$hP6$	$P6/mmm$	$E1_b$	$AgAuTe_4$ (sylvanite)	$mP12$	$P2/c$
$D2_e$	$BaHg_{11}$	$cP36$	$Pm\bar{3}m$	$E1_1$	$CuFeS_2$ (chalcopyrite)	$tI16$	$I\bar{4}2d$
$D2_f$	UB_{12}	$cF52$	$Fm\bar{3}m$	$E2_1$	$CaTiO_3$ (perovskite)	$cP5$	$Pm\bar{3}m$
$D2_g$	Fe_8N	$tI18$	$I4/mmm$	$E3$	Al_2CdS_4	$tI14$	$I\bar{4}$
$D2_h$	Al_6Mn	$oC28$	$Cmcm$	$E9_a$	Al_7Cu_2Fe	$tP40$	$P4/mnc$
$D2_1$	CaB_6	$cP7$	$Pm\bar{3}m$	$E9_b$	$Al_8FeMg_3Si_6$	$hP18$	$P\bar{6}2m$
$D2_3$	$NaZn_{13}$	$cF112$	$Fm\bar{3}c$	$E9_c$	Mn_3Al_9Si	$hP26$	$P6_3/mmc$
$D5_a$	Si_2U_3	$tP10$	$P4/mbm$	$E9_d$	$AlLi_3N_2$	$cI96$	$Ia\bar{3}$
$D5_b$	Pt_2Sn_3	$hP10$	$P6_3/mmc$	$E9_e$	$CuFe_2S_3$ (cubanite)	$oP24$	$Pnma$
$D5_c$	Pu_2C_3	$cI40$	$I\bar{4}3d$	$E9_3$	Fe_3W_3C (η carbide)	$cF112$	$Fd\bar{3}m$
$D5_e$	Ni_3S_2	$hR5$	$R32$	$E9_4$	Al_4C_4Si	$hP18$	$P6_3mc$
$D5_f$	As_2S_3	$mP20$	$P2_1/c$	$F0_1$	$NiSbS$ (ullmanite)	$cP12$	$P2_13$
$D5_1$	αAl_2O_3 (corundum)	$hR10$	$R\bar{3}c$	$F5_a$	$FeKS_2$	$mC16$	$C2/c$
$D5_2$	La_2O_3	$hP5$	$P\bar{3}m1$	$F5_1$	$NaCrS_2$	$hR4$	$R\bar{3}m$
$D5_3$	Mn_2O_3	$cI80$	$Ia\bar{3}$	$F5_6$	CuS_2Sb (wolfsbergite)	$oP16$	$Pnma$
$D5_4$	Sb_2O_3 (senarmontite)	$cF80$	$Fd\bar{3}m$	$H1_1$	Al_2MgO_4 (spinel)	$cF56$	$Fd\bar{3}m$
$D5_8$	Sb_2S_3	$oP20$	$Pnma$	$H2_4$	Cu_3VS_4 (sulvanite)	$cP8$	$P\bar{4}3m$
$D5_9$	Zn_3P_2	$tP40$	$P4_2/nmc$	$H2_6$	Cu_2FeSnS_4	$tI16$	$I\bar{4}2m$
$D5_{10}$	Cr_3C_2	$oP20$	$Pnma$	$L'1$	Fe_4N	$cP5$	$Pm\bar{3}m$
$D5_{11}$	Sb_2O_3 (valentinite)	$oP20$	$Pccn$	$L'1_2$	$AlFe_3C$ (perovskite)	$cP5$	$Pm\bar{3}m$
$D5_{13}$	Ni_2Al_3	$hP5$	$P\bar{3}m1$	$L'2_b$	ThH_2	$tI6$	$I4/mmm$
$D7_a$	δNi_3Sn_4	$mC14$	$C2/m$	$L'3$	Fe_2N	$hP3$	$P6_3/mmc$
$D7_b$	Ta_3B_4	$oI14$	$Immm$	$L1_a$	$CuPt_3$	$cF32$	$Fm\bar{3}c$
$D7_1$	Al_4C_3	$hR7$	$R\bar{3}m$	$L1_0$	$AuCu$	$tP4$	$P4/mmm$
$D7_2$	Co_3S_4	$cF56$	$Fd\bar{3}m$	$L1_1$	$CuPt$	$hR32$	$R\bar{3}m$
$D7_3$	Th_3P_4	$cI28$	$I\bar{4}3d$	$L1_2$	$AuCu_3$	$cP4$	$Pm\bar{3}m$
$D8_a$	$Mn_{23}Th_6$, $Cu_{16}Mg_6Si_7$ (G-phase)	$cF116$	$Fm\bar{3}m$	$L2_a$	$\delta CuTi$	$tP2$	$P4/mmm$
$D8_b$	$\sigma CrFe$	$tP30$	$P4_2/mnm$	$L2_1$	$AlCu_2Mn$ (Heusler)	$cF16$	$Fm\bar{3}m$
$D8_c$	Mg_2Zn_{11}	$cP39$	$Pm\bar{3}$	$L2_2$	Sb_2Tl_7	$cI54$	$Im\bar{3}m$
				$L6_0$	$CuTi_3$	$tP4$	$P4/mmm$

Appendix B - The back-propagation Algorithm - a mathematical approach

Units are connected to one another. Connections correspond to the edges of the underlying directed graph. There is a real number associated with each connection, which is called the weight of the connection. We denote by W_{ij} the weight of the connection from unit u_i to unit u_j. It is then convenient to represent the pattern of connectivity in the network by a weight matrix W whose elements are the weights W_{ij}. Two types of connection are usually distinguished: excitatory and inhibitory. A positive weight represents an excitatory connection whereas a negative weight represents an inhibitory connection. The pattern of connectivity characterises the architecture of the network.
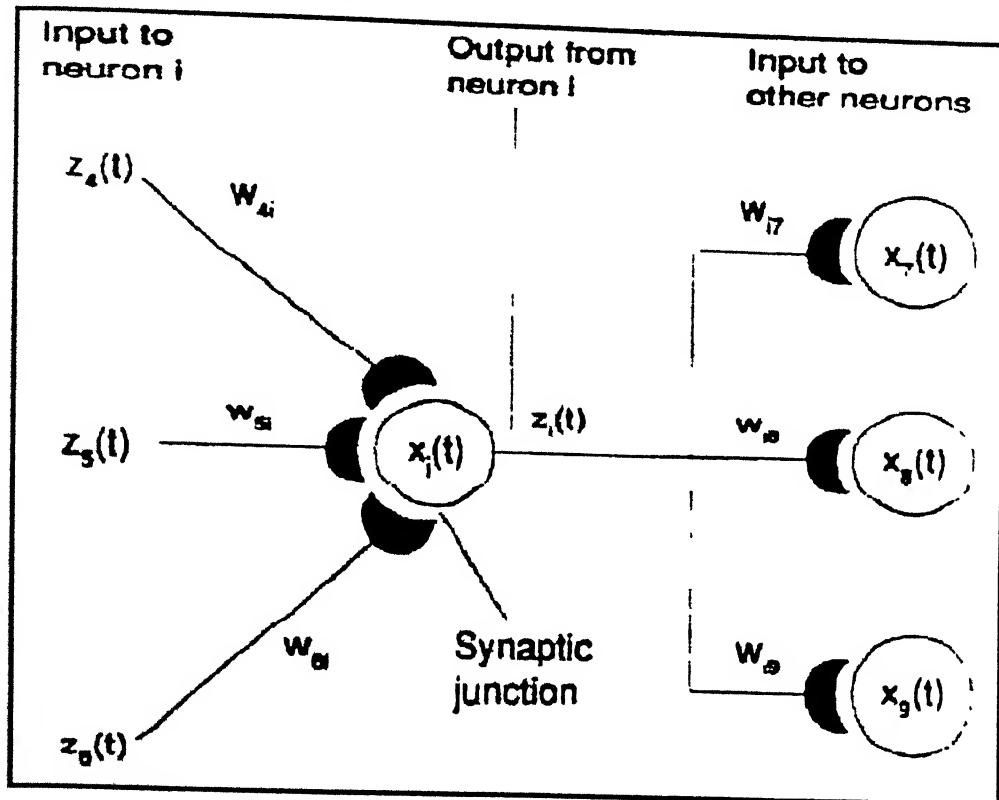
A unit in the output layer determines its activity by following a two step procedure.

● First, it computes the total weighted input x_j, using the formula:

$$X_j = \sum_i y_i W_{ij}$$

where y_i is the activity level of the jth unit in the previous layer and W_{ij} is the weight of the connection between the ith and the jth unit.

● Next, the unit calculates the activity y_j using some function of the total weighted input. Typically we use the sigmoid function:

$$y_j = \frac{1}{1 + e^{-x_j}}$$

Once the activities of all output units have been determined, the network computes the error E, which is defined by the expression:

1

where y_j is the activity level of the jth unit in the top layer and d_j is the desired output of the jth unit.

The back-propagation algorithm consists of four steps:

1. Compute how fast the error changes as the activity of an output unit is changed. This error derivative (EA) is the difference between the actual and the desired activity.

$$EA_j = \frac{\partial E}{\partial y_j} = y_j - d_j$$

2. Compute how fast the error changes as the total input received by an output unit is changed. This quantity (EI) is the answer from step 1 multiplied by the rate at which the output of a unit changes as its total input is changed.

$$EI_j = \frac{\partial E}{\partial x_j} = \frac{\partial E}{\partial y_j} \times \frac{dy_j}{dx_j} = EA_j y_j (1 - y_j)$$

3. Compute how fast the error changes as a weight on the connection into an output unit is changed. This quantity (EW) is the answer from step 2 multiplied by the activity level of the unit from which the connection emanates.

$$EW_{ij} = \frac{\partial E}{\partial W_{ij}} = \frac{\partial E}{\partial x_j} \times \frac{\partial x_j}{\partial W_{ij}} = EI_j y_i$$

4. Compute how fast the error changes as the activity of a unit in the previous layer is changed. This crucial step allows back propagation to be applied to multilayer networks. When the activity of a unit in the previous layer changes, it affects the activites of all the output units to which it is connected. So to compute the overall effect on the error, we add together all these seperate effects on output units. But each effect is simple to calculate. It is the answer in step 2 multiplied by the weight on the connection to that output unit.

$$EA_i = \frac{\partial E}{\partial y_i} = \sum_j \frac{\partial E}{\partial x_j} \times \frac{\partial x_j}{\partial y_i} = \sum_j EI_j W_{ij}$$

By using steps 2 and 4, we can convert the EAs of one layer of units into EAs for the previous layer. This procedure can be repeated to get the EAs for as many previous layers as desired. Once we know the EA of a unit, we can use steps 2 and 3 to compute the EWs on its incoming connections.